Construction of irreducible integrity basis for anisotropic hyperelasticity via structural tensors

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Abstract

We present a straightforward analytical-numerical methodology for determining polynomially complete and irreducible scalar-valued invariant sets for anisotropic hyperelasticity. By applying the proposed technique, we obtain irreducible integrity bases for all common anisotropies in hyperelasticity via the structural tensor concept, i.e., invariants are formed from a measure of deformation (symmetric 2nd order tensor) and a set of structural tensors describing the material's symmetry. Our work covers results for the 11 types of anisotropy that arise from the classical 7 crystal systems, as well as findings for 4 additional non-crystal anisotropies derived from the cylindrical, spherical, and icosahedral symmetry systems. Polynomial completeness and irreducibility of the proposed integrity bases are proven using the Molien series and, in addition, with established results for scalar-valued invariant sets from the literature. Furthermore, we derive relationships between a set of multiple structural tensors that specify a symmetry group and a description using only a single structural tensor. Both can be used to construct irreducible integrity bases by applying the proposed analytical-numerical method. The provided invariant sets are of great importance for modeling anisotropic materials via the structural tensor concept using both classical models as well as modern approaches based on machine learning. Alongside the results presented, this article also aims to provide an introductory overview of the complex field of modeling anisotropic materials.

Keywords anisotropic hyperelasticity · structural tensors · invariants · completeness and irreducibility · integrity bases · Molien series

1 Introduction

Materials such as composites or rolled metals are widely used in construction and engineering due to their direction-dependent mechanical responses, which arise from their internal structure. These anisotropic properties are deliberately exploited in fields like aerospace, automotive engineering, lightweight construction, and consumer product design to tailor characteristics such as stiffness and conductivity to specific performance requirements (Phiri et al., 2024).

In continuum theory, accurately capturing this behavior requires a constitutive model that sufficiently reflects the material's physical response. As Truesdell & Noll (1965) emphasized, formulating such models remains one of the central open problems in

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continuum mechanics. Many classical approaches (Chaimoon & Chindaprasirt, 2019, Holzapfel et al., 2000, 2005, May-Newman & Yin, 1998, Ogden & Saccomandi, 2007, Schröder et al., 2008, Wollner et al., 2023), as well as modern machine learning-based techniques such as neural networks (Dammaß et al., 2025a,b, Fuhg et al., 2022, Kalina et al., 2024a, Klein et al., 2022, Linden et al., 2023, Linka et al., 2021, Tac et al., 2022), rely on invariants as foundational elements of the model. These invariants encode material symmetry or anisotropy according to Neumann's principle, which states that the material symmetry must be preserved in the constitutive equations (Ebbing, 2010, Neumann & Meyer, 1885). Finding the relationships between specific anisotropies and the corresponding invariants was an important focus of research in the second half of the 20th century, during which various types of invariants were identified and classified in the context of continuum theory. Below, we provide a brief overview of some of the work done in this field.

1.1 Invariants for anisotropic materials

Smith & Rivlin (1958) initially computed invariants for the 32 point groups of the seven crystal systems leading to 11 out of 14 common anisotropies in hyperelasticity, which are presented in a so-called coordinate-dependent form. Shortly thereafter, Smith (1962) revisited these results and demonstrated that the invariants originally formulated by Smith & Rivlin (1958) form polynomially complete and irreducible sets or irreducible integrity bases. In subsequent works, this methodology was extended to include invariants for 1st and 2nd order tensors (Smith & Rivlin, 1964, Smith et al., 1963), enabling the formulation of constitutive models for coupled field problems such as magneto-mechanics (Eringen & Maugin, 1990, Kiral & Eringen, 1990). Although the invariants in Smith et al. (1963) were also classified as polynomially irreducible, Taurines et al. (2022) showed that one invariant associated with the cubic group O does not satisfy the criterion of polynomial irreducibility.

At the same time, numerous studies (Rivlin, 1955, Smith, 1960, 1965, 1970, 1971, Spencer, 1961, Spencer & Rivlin, 1958a,b, 1959, 1962, Wang, 1969a,b, 1970, 1971) have examined the determination of isotropic invariants. This line of work extended the consideration from individual tensors to arbitrary sets of 1st and 2nd order tensors. While Smith (1960, 1965), Spencer (1961), Spencer & Rivlin (1962) concentrated on irreducible integrity bases, Boehler (1977) provided a comprehensive summary of the developments of Smith (1970, 1971), Wang (1969a,b, 1970, 1971) and has formulated a general framework for constructing functional bases of isotropic invariants involving arbitrary sets of 1st order tensors as well as symmetric and antisymmetric 2nd order tensors. Pennisi & Trovato (1987) demonstrated that the formulation of Boehler (1977) also yields an irreducible functional basis for the isotropic case.

For the application to anisotropic cases, Lokhin & Sedov (1963) were the first to introduce the concept of structural tensors, which capture anisotropic properties through their invariance under specific symmetry transformations. Building on this idea, Zheng & Spencer (1993) showed that a single structural tensor is sufficient for capturing all symmetry properties of a specific group and provided explicit constructions for all relevant anisotropies. By incorporating these structural tensors as additional arguments into the constitutive functions, the results of Boehler (1977), Smith (1965) could be extended to derive integrity and functional bases for anisotropies described by structural tensors up to 2nd order. However, this approach was limited by the fact that, in some cases such as the hexagonal or cubic anisotropy, the tensor order of certain structural tensors exceeds two, with the exception of the triclinic, monoclinic, rhombic and cylindrical systems (Xiao et al., 2006). The work by Xiao (1996a) addressed this limitation by introducing structural tensor functions restricted to at most 2nd order, thereby enabling the computation of invariants for the remaining relevant anisotropies via the approach of Boehler (1977). Despite the fact that these invariants form a functional basis, they suffer from the crucial drawback of not being irreducible (functionally and polynomially) in general (Apel, 2004, Ebbing, 2010). Syzygies among the isotropic invariants of Boehler (1977), Smith (1965) stem from the fact that the structural tensors are constant. Nevertheless, this form of invariants is currently often used in research. For practical reasons, the often large number of resulting invariants is usually reduced by only considering those up to a specified polynomial degree (Apel, 2004, Ebbing, 2010, Kalina et al., 2024a).

Besides the works on integrity bases, numerous publications, such as Boehler (1979), Xiao (1995, 1996b, 1997a,b, 1998a,b,c,d), Xiao et al. (1999a,b, 2000a,b), have focused on the determination of functional bases in the anisotropic case, which typically contain a fewer number of invariants than the corresponding integrity bases. Finally, it is worth noting that there also exist studies addressing invariants of tensors of higher order than two such as Betten (1987), Ghosh et al. (2012), Itin (2016), Pennisi (1992).

1.2 Objectives and contributions of this work

As highlighted in the brief literature review, numerous results already exist on integrity bases for various anisotropies, some of which are proven to be polynomially irreducible (Smith, 1962). However, to the best of the authors' knowledge, irreducible integrity bases constituted by isotropic invariants and using structural tensors have not yet been established for all common anisotropies in hyperelasticity, which would be advantageous in the sense of minimal polynomial representations.

To address this gap, we present a straightforward analytical-numerical approach to extract irreducible integrity bases from a polynomially complete set of invariants. Applying this method within the framework of hyperelasticity, we demonstrate its effectiveness and, to the best of the authors' knowledge, provide for the first time irreducible integrity bases for all relevant anisotropies in finite strain elasticity using structural tensors, including the icosahedral symmetry group. In addition, alternative formulations of invariants based on different structural tensors are presented, along with the corresponding relationships between single and multiple structural tensors. As part of the validation process, reference is made to the properties of the Molien series as well as the coordinate-dependent irreducible integrity bases of Smith (1962).

Organization of this work In Sect. 2 we provide a brief introduction to strain and stress measures in continuum mechanics. Based on this, we give important requirements for hyperelastic potentials and summarize symmetry systems as well as point groups. Finally, this section introduces and compares the concepts of coordinate-dependent invariants and coordinate-free representation of invariants using structural tensors. In Sect. 3, we describe how an integrity basis can be obtained via isotropic extension and how irreducibility of the basis can be achieved by an analytical-numerical method. Two approaches for proving irreducibility of the integrity basis are presented thereafter. Afterwards we illustrate the methodology using a monoclinic and cubic anisotropy as examples. Sect. 4 then presents the calculated irreducible integrity bases for all anisotropies considered in this work. Finally, Sect. 5 summarizes the main advances for modeling the constitutive behavior of anisotropic materials and outlines directions for future research.

Definitions This work requires the introduction of specific terminology from mathematical subfields that are critical for an accurate description. To maintain the readability of the main text, these terms are compiled in A. Note that for clarity, we strictly distinguish between polynomial completeness and irreducibility, as well as functional completeness and irreducibility within the manuscript, cf. Remark 13.

Notation Generally, sets and tuples are denoted by calligraphic symbols, e.g., $\mathcal{S}$, $\mathcal{T}$. Blackboard bold symbols are used for domains of numbers: $\mathbb{Z}$, $\mathbb{Q}$ and $\mathbb{R}$ represent the sets of integers, rational, and real numbers, respectively. Any domain of number with a condition as a subscript consists only of elements that satisfy that condition. For example, $\mathbb{Z}_{\geq 0}$ denotes the set of positive integers, including zero. The space of nth order three-dimensional real-valued tensors is denoted by $\mathcal{L}^n$. Fully symmetric or skew-symmetric nth order tensors are elements of $\mathcal{L}^n_{\text{sym}}$ and $\mathcal{L}^n_{\text{skw}}$. We denote 0th, 1st, and 2nd order tensors as A, $\boldsymbol{A}$ and $\mathbf{A}$, respectively. To further simplify notation, we also use ${}^n\mathbf{A}$ for a tensor of arbitrary order $n \in \mathbb{Z}_{\geq 0}$. The single, double and quartic contraction between tensors are denoted by $\cdot$, $:$ and $::$, respectively. If tensors are directly adjacent to each other, such as ${}^n\mathbf{A}{}^m\mathbf{B} = {}^{n+m}\mathbf{C}$, this represents the dyadic product. In addition, the operator $\overset{m}{\otimes}{}^n\mathbf{A}$ stands for the m-fold dyadic product of ${}^n\mathbf{A}$, e.g., $\overset{3}{\otimes}\boldsymbol{A} = \boldsymbol{A}\boldsymbol{A}\boldsymbol{A}$, and ${}^n\mathbf{A}^m$ denotes the m-fold single contractions between each ${}^n\mathbf{A}$, e.g., $\mathbf{A}^3 = \mathbf{A}\cdot\mathbf{A}\cdot\mathbf{A}$. The cartesian basis vectors are denoted by $\boldsymbol{e}_i$, $i \in \{1, 2, 3\}$. In index notation, the coordinates of tensors are written with lower case Latin letters as subscripts, where Einstein's summation convention applies without restrictions if not stated otherwise. Furthermore, for groups (Def. 3) and rings (Def. 6) we use the same notation as for sets and tuples, e.g., group $\mathcal{G}$ and ring $\mathcal{R}$. The special orthogonal group as well as the orthogonal groups in three dimensions are denoted by $\mathcal{SO}(3)$ and $\mathcal{O}(3)$. Polynomial rings (Def. 7) in multiple variables x_μ and rings of $\mathcal{G}$-invariant polynomials are denoted by $\mathbb{R}[x_1, \ldots, x_k]$ and $\mathbb{R}_{\mathcal{G}}[x_1, \ldots, x_l]$, respectively. Thereby their field is the domain of real numbers $\mathbb{R}$. For reasons of readability, the arguments of functions are often omitted within this work. Furthermore, the symbol of a function is identical with the symbol of the function value itself in the following.

2 Fundamentals

2.1 Kinematics and stress measures

For finite deformations, a distinction is made between the reference configuration $\mathcal{B}_0 \subset \mathbb{R}^3$ at the initial time $\tau_0 \in \mathbb{R}$ and the current configuration $\mathcal{B}_\tau \subset \mathbb{R}^3$ at a time $\tau \geq \tau_0$. The smooth bijective and orientation preserving motion mapping $\boldsymbol{\varphi}_\tau : \mathcal{B}_0 \to \mathcal{B}_\tau$, $\boldsymbol{X} \mapsto \boldsymbol{\varphi}_\tau(\boldsymbol{X})$ maps each material point $\boldsymbol{X} \in \mathcal{B}_0$ from the reference configuration to the corresponding point $\boldsymbol{x}_\tau = \boldsymbol{\varphi}_\tau(\boldsymbol{X}) \in \mathcal{B}_\tau$ of the current configuration at time τ. In order to enable the calculation of derivatives w.r.t. time later on, we represent the mappings $\boldsymbol{\varphi}_\tau(\boldsymbol{X})$ as a function of space and time in what follows, i.e., $\boldsymbol{\varphi}(\boldsymbol{X}, \tau)$ (Šilhavý, 1997, Sect. 2.2). The deformation gradient $\mathbf{F} = (\nabla_{\boldsymbol{X}}\boldsymbol{\varphi})^\top \in \mathcal{L}^2$ with $\det \mathbf{F} > 0$, a so-called two-point tensor, is introduced as the central kinematic variable.[2] The deformation gradient $\mathbf{F} = \mathbf{R}\cdot\mathbf{U}$ can be multiplicatively decomposed into unique rotational part $\mathbf{R} \in \mathcal{SO}(3)$ and stretch part $\mathbf{U} \in \mathcal{L}^2_{\text{sym}}$. From that, the right Cauchy-Green deformation tensor $\mathbf{C} = \mathbf{F}^\top \cdot \mathbf{F} \in \mathcal{L}^2_{\text{sym}}$, which is objective and positive definite, and the Green-Lagrange strain tensor $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{1}) \in \mathcal{L}^2_{\text{sym}}$ can be calculated. These two quantities are related to the reference configuration and are therefore often referred to as Lagrangian or material strain measures.

[2] The coordinates of two-point 2nd order tensors are related to both reference and current configuration, e.g., the first coordinate of the deformation gradient $\mathbf{F} = F_{kl}\,\tilde{\boldsymbol{e}}_k\,\boldsymbol{e}_l$ is related to $\mathcal{B}_\tau$ whereas the second coordinate is related to $\mathcal{B}_0$, cf. (Marsden et al., 1984, Sect. 1.4), (Holzapfel, 2000, Sect. 2.4). Similar to $\mathbf{F}$, the 1st Piola-Kirchhoff stress tensor $\mathbf{P}$ is also a two-point tensor.

In addition to a variety of kinematic quantities, there are also several stress measures that can be introduced. Among the most important are the Cauchy stress tensor $\boldsymbol{\sigma} \in \mathcal{L}^2_{\text{sym}}$, the 1st Piola-Kirchhoff stress tensor $\mathbf{P} = J\boldsymbol{\sigma} \cdot \mathbf{F}^{-\top} \in \mathcal{L}^2$ and the 2nd Piola-Kirchhoff stress tensor $\mathbf{T} = J\mathbf{F}^{-1} \cdot \boldsymbol{\sigma} \cdot \mathbf{F}^{-\top} \in \mathcal{L}^2_{\text{sym}}$.

For a much more comprehensive introduction to continuum mechanics, please refer to the textbooks of Marsden et al. (1984), Šilhavý (1997) and Haupt (2000).

2.2 Conditions on hyperelastic potentials

An elastic constitutive model relates the deformation gradient to the stress induced at a material point. In hyperelasticity, this mapping is not defined directly, but via the scalar-valued Helmholtz free energy

$$\Psi : \mathcal{L}^2 \to \mathbb{R}_{\geq 0} , \ \mathbf{F} \mapsto \Psi(\mathbf{F}) \quad \text{and} \quad \mathbf{P} = \frac{\partial \Psi}{\partial \mathbf{F}} , \tag{1}$$

which ensures thermodynamic consistency to be effectively demonstrated using the Clausius–Duhem inequality by definition of $\mathbf{P}$ as the derivative with respect to $\mathbf{F}$ (Haupt, 2000, Holzapfel, 2000, Linden et al., 2023). Other key principles in constitutive modeling include determinism, the principle of equipresence and local action, objectivity as well as material symmetry.

The latter two principles are given by $\Psi\left(\mathbf{Q}_1 \cdot \mathbf{F} \cdot \mathbf{Q}_2^\top\right) = \Psi(\mathbf{F}) \ \forall \mathbf{Q}_1 \in \mathcal{SO}(3), \mathbf{Q}_2 \in \mathcal{G}$, where $\mathcal{G} \subseteq \mathcal{O}(3)$ is the symmetry group of the material. Thereby, setting $\mathbf{Q}_2 = \mathbf{1}$ isolates the requirement of objectivity, that is, invariance of the material behavior with respect to rigid body motions of the current configuration $\mathcal{B}_\tau$. By setting $\mathbf{Q}_1 = \mathbf{1}$, the requirement of material symmetry is isolated, i.e., invariance of the material behavior with respect to rigid body rotations $\mathbf{Q}_2 \in \mathcal{G}$ of the reference configuration $\mathcal{B}_0$. To guarantee objectivity, the Helmholtz free energy is expressed as a function of a deformation or strain measure that is objective. A common choice is $\Psi : \mathcal{L}^2 \to \mathbb{R}_{\geq 0} , \ \mathbf{C} \mapsto \Psi(\mathbf{C}(\mathbf{F}))$. In the following, we will pursue this approach and simply write $\Psi : \mathcal{L}^2_{\text{sym}} \to \mathbb{R}_{\geq 0} , \ \mathbf{C} \mapsto \Psi(\mathbf{C})$. As a consequence, merely the material symmetry condition in the form

$$\Psi\left(\mathbf{Q} \cdot \mathbf{C} \cdot \mathbf{Q}^\top\right) = \Psi(\mathbf{C}) \ \forall \mathbf{Q} \in \mathcal{G} \subseteq \mathcal{O}(3) \tag{2}$$

remains. In general, only some functions of $\mathbf{C}$ fulfill Eq. (2). These are called invariant functions, or simply invariants. Further constitutive conditions can be imposed on the elastic potential, such as the non-negativity of Ψ, which are explained in detail in Holzapfel et al. (2000) and Linden et al. (2023).

2.3 Overview on crystal classes and non-crystal classes

Many substances, both crystalline and non-crystalline, exhibit symmetry or geometric invariance with respect to certain rotations or roto-inversions. Therefore, we provide a brief overview of the symmetry systems relevant to this work.

Crystal systems A lot of materials, for example Diamond or Piypite, exhibit a special arrangement of their atoms, known as a crystal structure. The individual atoms are organized in a regular lattice, which consists of a periodic sequence of so-called unit cells. These cells are geometrically invariant to selected rotations represented by tensors $\mathbf{Q}_{\boldsymbol{p}}^{\varphi} \in \mathcal{SO}(3)$ and roto-inversions $-\mathbf{Q}_{\boldsymbol{p}}^{\varphi} \in \mathcal{O}(3)$, where $\boldsymbol{p} \in \mathcal{L}^2$ and $\varphi \in \mathbb{R}$ denote the axis and angle of rotation, respectively. All transformations, i.e., all rotations and roto-inversions, which lead to a microstructure that cannot be distinguished from the non-rotated configuration form a group $\mathcal{G} \subseteq \mathcal{O}(3)$ (Def. 3, Rem. 12).[3] The group is also referred to as a point group in materials science (Apel, 2004, Ebbing, 2010, Voigt, 1910). Such point groups are usually specified together with a set of generators (Def. 4) that generate all transformations against to which the unit cell is invariant. Furthermore, the point groups are categorized into seven crystal systems (Ebbing, 2010, Voigt, 1910): triclinic, monoclinic, rhombic, tetragonal, trigonal, hexagonal and cubic systems, containing the 32 point groups. In addition to one possible set of generators that clearly describes a group, the point groups are often specified by the Schoenflies notation or Hermann-Maugin notation. Here, we use the Schoenflies notation along with the designation $\mathcal{G}_i$ used by Zheng & Spencer (1993) to distinguish between the considered groups. In the context of hyperelasticity, some groups become equivalent due to the fact that the right Cauchy-Green deformation tensor $\mathbf{C}$ remains invariant under additional inversion of the transformation:

$$\tilde{\mathbf{C}} = \mathbf{Q}_{\boldsymbol{p}}^{\varphi} \cdot \mathbf{C} \cdot \left(\mathbf{Q}_{\boldsymbol{p}}^{\varphi}\right)^\top = -\mathbf{Q}_{\boldsymbol{p}}^{\varphi} \cdot \mathbf{C} \cdot \left(-\mathbf{Q}_{\boldsymbol{p}}^{\varphi}\right)^\top \quad \forall \, \mathbf{Q}_{\boldsymbol{p}}^{\varphi} \in \mathcal{SO}(3) . \tag{3}$$

Hence, transformations $\mathbf{Q}_{\boldsymbol{p}}^{\varphi} \in \mathcal{SO}(3)$ and $-\mathbf{Q}_{\boldsymbol{p}}^{\varphi} \in \mathcal{O}(3)$ are indistinguishable for $\mathbf{C}$ if they share the same axis and angle of rotation. We highlight this by introducing a third notation $\mathscr{A}_i$, representing a specific anisotropy in hyperelasticity. Tab. 1 provides an overview of the 32 crystallographic point groups, including the three notations used, a possible set of generators, and the group order (number of elements), denoted by $|\mathcal{G}|$.

[3] Independently of the specific microstructure, it can be verified that $(\mathcal{G}, \cdot)$ is indeed a group fulfilling the axioms of Def. 3 in straightforward manner: Single contraction of tensors is associative, the 2nd order identity tensor $\mathbf{1} \in \mathcal{L}^2_{\text{sym}}$ always is an element of $\mathcal{G}$ and $\mathbf{Q}_{\boldsymbol{p}}^{\varphi} \in \mathcal{G}$ implies $\left(\mathbf{Q}_{\boldsymbol{p}}^{\varphi}\right)^{-1} \in \mathcal{G}$.

It should be noted that, in addition to materials whose atomic structure leads to geometric invariance, materials like wood and rolled sheet metal can also be associated with one of the groups of the seven crystal systems.[4]

Remark 1. In the case of even-order tensors whose coordinates all refer to the same configuration, certain groups become equivalent due to the fact that such tensors are invariant under inversion of the transformation, regardless of existing symmetries. Thus, transformations $\mathbf{Q}_{\boldsymbol{p}}^{\varphi}$ and $-\mathbf{Q}_{\boldsymbol{p}}^{\varphi}$ are indistinguishable for such tensors. This property, however, does generally not hold for tensors of odd order and two-point tensors such as the deformation gradient $\mathbf{F}$, cf. Footnote 2.

Non-crystal systems Many materials, such as fiber-reinforced composites (Chatterjee & Kumar, 2025, Ehret & Itskov, 2007, Kalina et al., 2023, Lauff et al., 2025) or magnetorheological elastomers (Bustamante, 2010, Kalina et al., 2024b), exhibit geometric invariance under transformations that are not among the 32 crystallographic point groups. In this context, one speaks of non-crystal systems, of which there are infinitely many. Among the most important systems are the spherical (isotropic) and the cylindrical (transversal-isotropic), whose associated point groups have an infinite number of elements. However, not all groups associated with non-crystal systems contain an infinite number of elements. A notable example is the icosahedral system, which comprises two groups, each possessing a finite number of transformations. As with the crystal systems, several groups coincide in hyperelasticity due to the transformation properties of the 2nd order tensor $\mathbf{C}$, cf. Eq. (3). Consequently, the five groups of the cylindrical system reduce to two distinct anisotropies, and one additional anisotropy each arises from the spherical and icosahedral systems, respectively. Again, we use the Schoenflies notation, the notation of Zheng & Spencer (1993) and the anisotropy type $\mathscr{A}_i$ for the different groups of the non-crystal systems. It should be noted that Zheng & Spencer (1993) did not consider the spherical and icosahedral systems, which is why no notation is available in these cases. The point groups of the considered non-crystal systems are listed in Tab. 2.

2.4 Formulation of hyperelastic potentials with invariants

In continuum mechanics, material models are often formulated using deformation or strain tensors that ensure objectivity, see Sect. 2.2. To additionally guarantee material symmetry, the use of scalar-valued invariants is appealing. Therefore, we begin with a general definition of invariants within this framework. To this end, we first introduce the function

$$\star : \mathcal{G} \times \bigcup_{n\geq 0} \mathcal{L}^n \to \bigcup_{n\geq 0} \mathcal{L}^n, \quad \begin{cases} (\mathbf{Q}, H) \mapsto \mathbf{Q} \star H := H & n=0 \\ (\mathbf{Q}, \boldsymbol{H}) \mapsto \mathbf{Q} \star \boldsymbol{H} := \mathbf{Q}\cdot\boldsymbol{H} = H_i\,\mathbf{Q}\cdot\boldsymbol{e}_i & n=1 \\ (\mathbf{Q}, \mathbf{H}) \mapsto \mathbf{Q} \star \mathbf{H} := \mathbf{Q}\cdot\mathbf{H}\cdot\mathbf{Q}^{\top} = H_{i_1 i_2}\mathbf{Q}\cdot\boldsymbol{e}_{i_1}\mathbf{Q}\cdot\boldsymbol{e}_{i_2} & n=2 \\ (\mathbf{Q}, {}^{n}\mathbf{H}) \mapsto \mathbf{Q} \star {}^{n}\mathbf{H} := H_{i_1\ldots i_n}\mathbf{Q}\cdot\boldsymbol{e}_{i_1}\ldots\mathbf{Q}\cdot\boldsymbol{e}_{i_n} & n>2 \end{cases}, \quad \mathbf{Q}\in\mathcal{G}\,, \tag{4}$$

which provides a compact notation for describing the action of a group element $\mathbf{Q} \in \mathcal{G} \subseteq O(3)$ on tensors of arbitrary order, cf. Apel (2004), Xiao (1996a). In other words, $\star$ links the pair of transformation $\mathbf{Q}$ and an (untransformed) tensor ${}^{n}\mathbf{H}$ to the transformed match of ${}^{n}\mathbf{H}$. To further shorten the notation, the transformation of several tensors, that are gathered in a tuple $\mathcal{H}_{\mathcal{G}} = ({}^{n_1}\mathbf{H}_1, \ldots, {}^{n_k}\mathbf{H}_k)$, $k \in \mathbb{Z}_{\geq 1}$, by the same group element $\mathbf{Q} \in \mathcal{G}$ is denoted by

$$\mathbf{Q} \star \mathcal{H}_{\mathcal{G}} := (\mathbf{Q} \star {}^{n_1}\mathbf{H}_1, \ldots, \mathbf{Q} \star {}^{n_k}\mathbf{H}_k)\ . \tag{5}$$

Definition 1 (Scalar invariant)**.** Let $I : \mathcal{L}^{n_1} \times \cdots \times \mathcal{L}^{n_k} \to \mathbb{R}$, $\mathcal{H}_{\mathcal{G}} \mapsto I(\mathcal{H}_{\mathcal{G}})$ be a scalar-valued function of k tensors ${}^{n_\lambda}\mathbf{H}_\lambda$, gathered in the tuple $\mathcal{H}_{\mathcal{G}} = ({}^{n_1}\mathbf{H}_1, \ldots, {}^{n_k}\mathbf{H}_k)$, $k \in \mathbb{Z}_{>0}, n_1, \ldots, n_k \in \mathbb{Z}_{\geq 0}$. The scalar-valued function $I(\mathcal{H}_{\mathcal{G}})$ is called invariant under the group $\mathcal{G} \subseteq O(3)$, $\mathcal{G}$-invariant or simply invariant, if it satisfies the condition

$$I(\mathcal{H}_{\mathcal{G}}) = I(\mathbf{Q} \star \mathcal{H}_{\mathcal{G}}) \quad \forall\, \mathbf{Q} \in \mathcal{G}\,. \tag{6}$$

Note that the concept of invariants, in general, does not need to be limited to scalar-valued functions (Zheng, 1994). However, scalar invariants are of particular relevance for formulating scalar-valued energy potentials, and we therefore restrict our focus to this scenario throughout the paper.

For any group $\mathcal{G} \subseteq O(3)$, there exists an infinite number of scalar-valued invariants, which can be algebraic, rational, polynomial or homogeneous polynomial functions. As shown by Spencer (1971), it is useful to focus on homogeneous polynomial invariants. This is because algebraic invariants are solutions of algebraic equations with the coefficients being rational invariants. Furthermore, these rational invariants can be written as ratios of polynomial invariants, which can be expressed as a sum of homogeneous polynomial invariants, respectively. Consequently, it becomes essential to identify a finite subset of homogeneous polynomial invariants from which all other $\mathcal{G}$-invariant polynomials can be expressed as a polynomial function in the elements of that subset. Such a set is referred to as polynomially complete (Def. 9) or an integrity basis (Def. 14). If, in addition, none of the invariants in this set can be expressed as a polynomial function of the others, the set is termed polynomially irreducible (Def. 10). The elements of a polynomially complete and irreducible set or an irreducible integrity basis are called fundamental invariants (Def. 11). While an irreducible integrity basis is not unique, the number of fundamental invariants with a given polynomial degree is fixed. Note that the concepts introduced require to consider algebraic structures and their properties, such as polynomial rings (Def. 7) and rings of invariant polynomials (Def. 8).

[4]Because of the non-straight grain direction in wood, the orientation of the symmetry transformations varies. However, for arbitrarily small volume elements, wood can still be classified as rhombic.

Table 1: The 32 finite point groups of the seven crystal systems, inspired by Apel (2004), Smith et al. (1963), Zheng & Spencer (1993). The Schoenflies symbols and the designations according to Zheng & Spencer (1993) are provided, along with the various types of anisotropy encountered in hyperelasticity. $\boldsymbol{x}$, $\boldsymbol{y}$, $\boldsymbol{z}$ and $\boldsymbol{k}$ denote the x-, y-, z- and $[\boldsymbol{k}] = 1/\sqrt{3}\,(-1,-1,-1)^\top$-axis.

Crystal system	Point group	Schoenflies	Zheng/Spencer	Anisotropy type	$\lvert\mathcal{G}\rvert$	Generators
triclinic	pedial	$\mathcal{C}_1$	$\mathcal{G}_1$	$\mathscr{A}_1$	1	$\mathbf{1}$
	pinacoidal	$\mathcal{C}_i$ / $\mathcal{S}_2$	$\mathcal{G}_2$	$\mathscr{A}_1$	2	$-\mathbf{1}$
monoclinic	sphenoidal	$\mathcal{C}_2$	$\mathcal{G}_4$	$\mathscr{A}_2$	2	$\mathbf{Q}_{\boldsymbol{z}}^{\pi}$
	domatic	$\mathcal{C}_{1h}$	$\mathcal{G}_3$	$\mathscr{A}_2$	2	$-\mathbf{Q}_{\boldsymbol{z}}^{\pi}$
	prismatic	$\mathcal{C}_{2h}$	$\mathcal{G}_5$	$\mathscr{A}_2$	4	$-\mathbf{1}, \mathbf{Q}_{\boldsymbol{z}}^{\pi}$
rhombic	rhombic-disphenoidal	$\mathcal{D}_2$	$\mathcal{G}_7$	$\mathscr{A}_3$	4	$\mathbf{Q}_{\boldsymbol{z}}^{\pi}, \mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	rhombic-pyramidal	$\mathcal{C}_{2v}$	$\mathcal{G}_6$	$\mathscr{A}_3$	4	$\mathbf{Q}_{\boldsymbol{z}}^{\pi}, -\mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	rhombic-dipyramidal	$\mathcal{D}_{2h}$	$\mathcal{G}_8$	$\mathscr{A}_3$	8	$-\mathbf{1}, \mathbf{Q}_{\boldsymbol{z}}^{\pi}, \mathbf{Q}_{\boldsymbol{x}}^{\pi}$
tetragonal	tetragonal-pyramidal	$\mathcal{C}_4$	$\mathcal{G}_{10}$	$\mathscr{A}_4$	4	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}$
	tetragonal-disphenoidal	$\mathcal{C}_{2i}$ / $\mathcal{S}_4$	$\mathcal{G}_9$	$\mathscr{A}_4$	4	$-\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}$
	tetragonal-dipyramidal	$\mathcal{C}_{4h}$	$\mathcal{G}_{11}$	$\mathscr{A}_4$	8	$-\mathbf{1}, \mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}$
	tetragonal-trapezohedral	$\mathcal{D}_4$	$\mathcal{G}_{14}$	$\mathscr{A}_5$	8	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}, \mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	ditetragonal-pyramidal	$\mathcal{C}_{4v}$	$\mathcal{G}_{13}$	$\mathscr{A}_5$	8	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}, -\mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	tetragonal-scalenohedral	$\mathcal{D}_{2d}$	$\mathcal{G}_{12}$	$\mathscr{A}_5$	8	$-\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}, -\mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	ditetragonal-dipyramidal	$\mathcal{D}_{4h}$	$\mathcal{G}_{15}$	$\mathscr{A}_5$	16	$-\mathbf{1}, \mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}, \mathbf{Q}_{\boldsymbol{x}}^{\pi}$
trigonal	trigonal-pyramidal	$\mathcal{C}_3$	$\mathcal{G}_{16}$	$\mathscr{A}_6$	3	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{2\pi}{3}}$
	rhombohedral	$\mathcal{C}_{3i}$ / $\mathcal{S}_6$	$\mathcal{G}_{17}$	$\mathscr{A}_6$	6	$-\mathbf{Q}_{\boldsymbol{z}}^{\frac{2\pi}{3}}$
	trigonal-trapezohedral	$\mathcal{D}_3$	$\mathcal{G}_{19}$	$\mathscr{A}_7$	6	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{2\pi}{3}}, \mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	ditrigonal-pyramidal	$\mathcal{C}_{3v}$	$\mathcal{G}_{18}$	$\mathscr{A}_7$	6	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{2\pi}{3}}, -\mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	hexagonal-scalenohedral	$\mathcal{D}_{3d}$	$\mathcal{G}_{20}$	$\mathscr{A}_7$	12	$-\mathbf{Q}_{\boldsymbol{z}}^{\frac{2\pi}{3}}, \mathbf{Q}_{\boldsymbol{x}}^{\pi}$
hexagonal	hexagonal-pyramidal	$\mathcal{C}_6$	$\mathcal{G}_{22}$	$\mathscr{A}_8$	6	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{3}}$
	trigonal-dipyramidal	$\mathcal{C}_{3h}$	$\mathcal{G}_{21}$	$\mathscr{A}_8$	6	$-\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{3}}$
	hexagonal-dipyramidal	$\mathcal{C}_{6h}$	$\mathcal{G}_{23}$	$\mathscr{A}_8$	12	$-\mathbf{1}, \mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{3}}$
	hexagonal-trapezohedral	$\mathcal{D}_6$	$\mathcal{G}_{26}$	$\mathscr{A}_9$	12	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{3}}, \mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	dihexagonal-pyramidal	$\mathcal{C}_{6v}$	$\mathcal{G}_{25}$	$\mathscr{A}_9$	12	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{3}}, -\mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	ditrigonal-dipyramidal	$\mathcal{D}_{3h}$	$\mathcal{G}_{24}$	$\mathscr{A}_9$	12	$-\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{3}}, -\mathbf{Q}_{\boldsymbol{x}}^{\pi}$
	dihexagonal-dipyramidal	$\mathcal{D}_{6h}$	$\mathcal{G}_{27}$	$\mathscr{A}_9$	24	$-\mathbf{1}, \mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{3}}, \mathbf{Q}_{\boldsymbol{x}}^{\pi}$
cubic	tetartoidal	$\mathcal{T}$	$\mathcal{G}_{28}$	$\mathscr{A}_{10}$	12	$\mathbf{Q}_{\boldsymbol{z}}^{\pi}, \mathbf{Q}_{\boldsymbol{k}}^{\frac{2\pi}{3}}$
	diploidal	$\mathcal{T}_h$	$\mathcal{G}_{29}$	$\mathscr{A}_{10}$	24	$\mathbf{Q}_{\boldsymbol{z}}^{\pi}, -\mathbf{Q}_{\boldsymbol{k}}^{\frac{2\pi}{3}}$
	gyroidal	$\mathcal{O}$	$\mathcal{G}_{31}$	$\mathscr{A}_{11}$	24	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}, \mathbf{Q}_{\boldsymbol{x}}^{\frac{\pi}{2}}$
	hextetrahedral	$\mathcal{T}_d$	$\mathcal{G}_{30}$	$\mathscr{A}_{11}$	24	$-\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}, -\mathbf{Q}_{\boldsymbol{x}}^{\frac{\pi}{2}}$
	hexoctahedral	$\mathcal{O}_h$	$\mathcal{G}_{32}$	$\mathscr{A}_{11}$	48	$\mathbf{Q}_{\boldsymbol{z}}^{\frac{\pi}{2}}, -\mathbf{Q}_{\boldsymbol{k}}^{\frac{2\pi}{3}}$

Table 2: Point groups of the cylindrical, spherical and icosahedral system, inspired by Apel (2004). For the Schoenflies symbols, the designations according to Zheng & Spencer (1993) are provided, along with the various types of anisotropy encountered in hyperelasticity. $\boldsymbol{x}$, $\boldsymbol{z}$ denote the x-, z-axis. $[\boldsymbol{g}] = 1/\sqrt{\tau^2 - 2\tau + 2}\,(\tau - 1, 0, 1)^\top$ with the golden ratio $\tau = (1 + \sqrt{5})/2$ and $[\boldsymbol{p}] = 1/\sqrt{3}\,(1, 1, 1)^\top$.

Non crystal system	Schoenflies	Zheng/Spencer	Anisotropy type	$\lvert\mathcal{G}\rvert$	Generators
cylindrical	$\mathcal{C}_\infty$ / $\mathcal{T}_1$	$\mathcal{T}_1$	$\mathscr{A}_{12}$	∞	$\mathbf{Q}_z^\gamma$, $\gamma \in [0, 2\pi)$
	$\mathcal{C}_{\infty h}$ / $\mathcal{T}_3$	$\mathcal{T}_3$	$\mathscr{A}_{12}$	∞	$-\mathbf{1}, \mathbf{Q}_z^\gamma$, $\gamma \in [0, 2\pi)$
	$\mathcal{D}_\infty$ / $\mathcal{T}_5$	$\mathcal{T}_5$	$\mathscr{A}_{13}$	∞	$\mathbf{Q}_z^\gamma, \mathbf{Q}_x^\pi$, $\gamma \in [0, 2\pi)$
	$\mathcal{C}_{\infty v}$ / $\mathcal{T}_2$	$\mathcal{T}_2$	$\mathscr{A}_{13}$	∞	$\mathbf{Q}_z^\gamma, -\mathbf{Q}_x^\pi$, $\gamma \in [0, 2\pi)$
	$\mathcal{D}_{\infty h}$ / $\mathcal{T}_4$	$\mathcal{T}_4$	$\mathscr{A}_{13}$	∞	$-\mathbf{1}, \mathbf{Q}_z^\gamma, \mathbf{Q}_x^\pi$, $\gamma \in [0, 2\pi)$
spherical	$\mathcal{K}$ / $\mathcal{SO}(3)$	-	$\mathscr{A}_{14}$	∞	$\mathbf{Q}_z^\gamma, \mathbf{Q}_x^\alpha$, $\gamma, \alpha \in [0, 2\pi)$
	$\mathcal{K}_h$ / $\mathcal{O}(3)$	-	$\mathscr{A}_{14}$	∞	$-\mathbf{1}, \mathbf{Q}_z^\gamma, \mathbf{Q}_x^\alpha$, $\gamma, \alpha \in [0, 2\pi)$
icosahedral	$\mathcal{I}$	-	$\mathscr{A}_{15}$	60	$\mathbf{Q}_{\boldsymbol{g}}^{\frac{2\pi}{5}}, \mathbf{Q}_{\boldsymbol{p}}^{\frac{2\pi}{3}}$
	$\mathcal{I}_h$	-	$\mathscr{A}_{15}$	120	$\mathbf{Q}_{\boldsymbol{g}}^{\frac{2\pi}{5}}, -\mathbf{Q}_{\boldsymbol{p}}^{\frac{2\pi}{3}}$

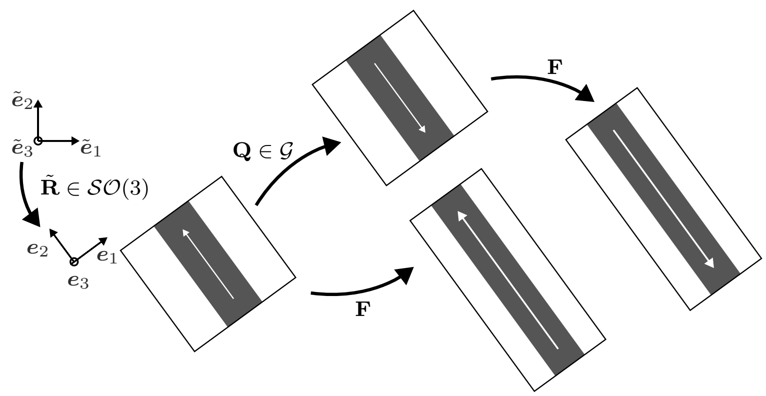

Figure 1: Principle of material symmetry using coordinate-dependent invariants. The use of invariants in coordinate-dependent form requires specification in a fixed reference frame, as the orientation of the transformation $\mathbf{Q} \in \mathcal{G}$ is predefined. Therefore, a preliminary coordinate transformation using $\tilde{\mathbf{R}} \in \mathcal{SO}(3)$ is necessary to ensure that the reference frame $\tilde{\boldsymbol{e}}_i$ coincides with that of the invariants $\boldsymbol{e}_i$.

2.4.1 Invariants in coordinate-dependent form

In the context of hyperelasticity, Smith & Rivlin (1958) were the first to compute integrity bases for all anisotropy types arising from the point groups of the crystal systems. Smith (1962) also proved that the identified integrity bases are indeed polynomially complete and irreducible. This represents a significant advantage as it ensures that the number of invariants in terms of polynomial representation is the minimum. The irreducible integrity bases determined by Smith (1962) are listed in D.

Although these invariants are invariant under all transformations of a given group, as defined by Eq. (6), they also require a fixed orientation of the reference coordinate system. We refer to such invariants as coordinate-dependent invariants. To apply this concept using Def. 1, we define $\mathcal{H}_\mathcal{G} = (\mathbf{C})$.[5] Before coordinate-dependent invariants can be used in a model, the reference frame of the constitutive variable must be aligned with that of the invariants, which is denoted in terms of the tensor $\mathbf{C}$ as

$$I([C_{ij}]) = I([\tilde{R}_{ik}\tilde{R}_{jl}\tilde{C}_{kl}]), \quad \tilde{\mathbf{R}} \in \mathcal{SO}(3)\ , \tag{7}$$

where the notation $[C_{ij}]$ denotes the coordinates of the tensor given in a 3×3 matrix. The necessary passive rotation $\tilde{\mathbf{R}}$ in context of material symmetry is illustrated in Fig. 1.

2.4.2 Structural tensor concept

A completely different approach is the structural tensor concept, which is favored in modern work (Apel, 2004, Bustamante, 2010, Ciambella et al., 2024, Ehret & Itskov, 2007, Holthusen & Kuhl, 2025, Kalina et al., 2024a, Klein et al., 2022, Ogden &

[5]Any suitable deformation or strain measure may be used instead of the right Cauchy-Green deformation tensor $\mathbf{C} \in \mathcal{L}^2_{\text{sym}}$, as long as it is a symmetric second order tensor, which is not a two-point tensor. For example, the invariants of the Green-Lagrange strain tensor $\mathbf{E} \in \mathcal{L}^2_{\text{sym}}$ have exactly the same form as those formulated in $\mathbf{C}$.

Saccomandi, 2007, Reese et al., 2021, Schröder & Neff, 2003, Wollner et al., 2023) and can be traced back to the work of Lokhin & Sedov (1963). The idea is that the list of arguments of the potential Ψ is extended by a tuple

$$\mathcal{M}_{\mathcal{G}} = ({}^{n_1}\mathbf{M}_1, \dots, {}^{n_l}\mathbf{M}_l) \tag{8}$$

of $l \in \mathbb{Z}_{\geq 1}$ structural tensors ${}^{n_\mu}\mathbf{M}_\mu \in \mathcal{L}^{n_\mu}$ to obtain scalar-valued isotropic tensor functions. The structural tensors are related to the reference configuration $\mathcal{B}_0$ and describe the material's underlying symmetry.[6]

Invariance of structural tensors Let us now consider how the structural tensors behave under orthogonal transformations. Since they describe the underlying material symmetry in the reference configuration $\mathcal{B}_0$, this can be interpreted as a rotation of $\mathcal{B}_0$.

If the tuple $\mathcal{M}_{\mathcal{G}}$ includes only a single structural tensor ${}^{n}\mathbf{M}$, this tensor always has to satisfy the conditions

$${}^{n}\mathbf{M} = \mathbf{Q} \star {}^{n}\mathbf{M} \;\forall\, \mathbf{Q} \in \mathcal{G} \subseteq \mathcal{O}(3) \quad \wedge \quad {}^{n}\mathbf{M} \neq \mathbf{Q} \star {}^{n}\mathbf{M} \;\forall\, \mathbf{Q} \notin \mathcal{G} \subseteq \mathcal{O}(3)\,, \tag{9}$$

thereby completely capturing the anisotropy of a material, which is equivalent to ${}^{n}\mathbf{M} = \mathbf{Q} \star {}^{n}\mathbf{M} \Leftrightarrow \mathbf{Q} \in \mathcal{G} \subseteq \mathcal{O}(3)$.

In the more general case, the tuple $\mathcal{M}_{\mathcal{G}}$ consists of multiple structural tensors. Then each tensor

$${}^{n_\mu}\mathbf{M}_\mu = \mathbf{Q} \star {}^{n_\mu}\mathbf{M}_\mu \;\forall\, \mathbf{Q} \in \mathcal{G} \subseteq \mathcal{O}(3) \tag{10}$$

must at least be invariant under all transformations of a given group $\mathcal{G} \subseteq \mathcal{O}(3)$, i.e., ${}^{n_\mu}\mathbf{M}_\mu$ can therefore also be invariant with respect to transformations $\mathbf{Q} \notin \mathcal{G}$ that are not contained in the symmetry group and not only to the ones included in $\mathcal{G}$. However, considered as a whole, the set of transformations that leave all structural tensors ${}^{n_\mu}\mathbf{M}_\mu$ (i.e., for all $\mu \in \{1, \dots, l\}$) invariant must coincide with the group $\mathcal{G}$. Hence, the conditions

$$\mathcal{M}_{\mathcal{G}} = \mathbf{Q} \star \mathcal{M}_{\mathcal{G}} \;\forall\, \mathbf{Q} \in \mathcal{G} \subseteq \mathcal{O}(3) \quad \wedge \quad \mathcal{M}_{\mathcal{G}} \neq \mathbf{Q} \star \mathcal{M}_{\mathcal{G}} \;\forall\, \mathbf{Q} \notin \mathcal{G} \subseteq \mathcal{O}(3) \tag{11}$$

follow for the entire tuple of structural tensors.

Isotropic extension of the elastic potential By using the tuple of structural tensors as additional arguments in the free energy, an anisotropic elastic potential $\Psi(\mathbf{C})$ is replaced by a scalar-valued isotropic tensor function

$$\Psi : \mathcal{L}^2_{\text{sym}} \times \mathcal{L}^{n_1} \times \dots \times \mathcal{L}^{n_\mu} \times \dots \mathcal{L}^{n_l} \to \mathbb{R}_{\geq 0}\,, \; (\mathbf{C}, \mathcal{M}_{\mathcal{G}}) \mapsto \Psi\left(\mathbf{C}, \mathcal{M}_{\mathcal{G}}\right) \tag{12}$$

of multiple arguments, with $n_\mu \in \mathbb{Z}_{\geq 1}$ for all $\mu \in \{1, \dots, l\}$. Thus, the material symmetry condition (2) becomes

$$\Psi\left(\mathbf{Q} \star \mathbf{C}, \mathbf{Q} \star \mathcal{M}_{\mathcal{G}}\right) = \Psi\left(\mathbf{C}, \mathcal{M}_{\mathcal{G}}\right) \;\forall\, \mathbf{Q} \in \mathcal{O}(3)\,. \tag{13}$$

This procedure is also known as isotropic extension (Apel, 2004, Xiao, 1996a).

In order to clearly analyze the connection to the movement of a body, let us now consider the energy density $\Psi\left(\mathbf{F}, \mathcal{M}_{\mathcal{G}}\right)$ for which we find $\Psi\left(\mathbf{F}, \mathcal{M}_{\mathcal{G}}\right) = \Psi\left(\mathbf{F} \cdot \mathbf{Q}^\top, \mathbf{Q} \star \mathcal{M}_{\mathcal{G}}\right) \;\forall\, \mathcal{SO}(3)$. Based on this, Fig. 2 provides a visual representation of this relationship: First, the body is rotated by an arbitrary $\mathbf{Q} \in \mathcal{SO}(3)$ and thus the structural tensors are actively transformed by $\mathbf{Q} \star \mathcal{M}_{\mathcal{G}}$. Then, the deformation $\mathbf{F} \cdot \mathbf{Q}^\top$ is applied, where $\mathbf{Q}^\top$ rotates the body in the opposite direction, thereby restoring the original non-rotated configuration for all $\mathbf{Q} \in \mathcal{SO}(3)$, and afterwards $\mathbf{F}$ is applied. This is therefore the same as if we directly apply the deformation $\mathbf{F}$ to the non-rotated configuration with the non-transformed tuple of structural tensors $\mathcal{M}_{\mathcal{G}}$. As a result, including $\mathcal{M}_{\mathcal{G}}$ ensures that $\Psi\left(\mathbf{F}, \mathcal{M}_{\mathcal{G}}\right)$ is an isotropic tensor function. The same holds for $\Psi\left(\mathbf{C}, \mathcal{M}_{\mathcal{G}}\right)$.

Invariants with structural tensors To formulate the elastic potential, invariants of $\mathbf{C}$ and $\mathcal{M}_{\mathcal{G}}$, so-called isotropic invariants, are formed. Thus, the tuple $\mathcal{H}_{\mathcal{G}}$ used in Def. 1 is specified below by the chosen constitutive variable and the structural tensors as $\mathcal{H}_{\mathcal{O}(3)}$.

Definition 2 (Isotropic invariant)**.** An invariant I, which obeys the condition

$$I(\mathcal{H}_{\mathcal{O}(3)}) = I(\mathbf{Q} \star \mathcal{H}_{\mathcal{O}(3)}) \quad \forall\, \mathbf{Q} \in \mathcal{O}(3)\,, \tag{14}$$

is called isotropic invariant.

[6] As is common practice, we define the push-forward of the structural tensors onto the current configuration $\mathcal{B}_\tau$ using the rotational part $\mathbf{R} \in \mathcal{SO}(3)$ of $\mathbf{F} = \mathbf{R} \cdot \mathbf{U}$, i.e., by $\mathbf{R} \star {}^{n_\mu}\mathbf{M}_\mu$. This can be understood to mean that only the change in orientation during the transformation plays a role. With this choice of the push-forward, norms of structural tensors or (generalized) traces of structural tensors of even degree also remain constant. However, the push-forward operation is usually not necessary, since the constitutive equations are typically formulated with $\mathbf{C}$, which is related to the reference.

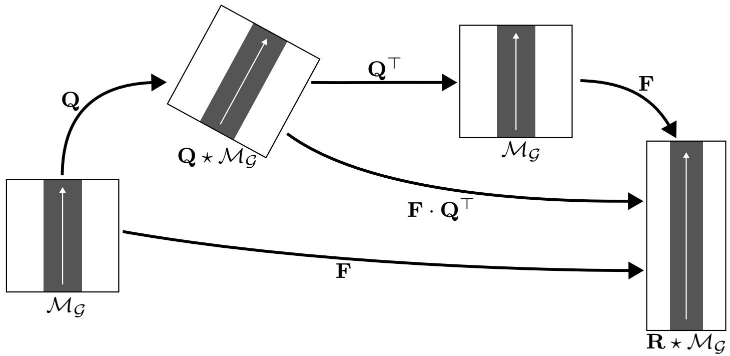

Figure 2: Illustration of the structural tensor concept for obtaining isotropic tensor functions. The material is actively rotated by applying the transformation $\mathbf{Q} \in \mathcal{O}(3)$ to the structural tensors in $\mathcal{M}_\mathcal{G}$. This rotation is then reversed using $\mathbf{Q}^\top$, thereby ensuring that the principle of material symmetry is satisfied $\forall\, \mathbf{Q} \in \mathcal{O}(3)$. $\mathbf{R} = \mathbf{F} \cdot \mathbf{U}^{-1}$ denotes the rotational component of the deformation gradient.

In hyperelasticity, $\mathcal{H}_{\mathcal{O}(3)}$ consists of a constitutive variable, such as $\mathbf{C}$, and one or multiple structural tensors gathered in the tuple $\mathcal{M}_\mathcal{G}$, i.e., $\mathcal{H}_{\mathcal{O}(3)} = (\mathbf{C}, {}^{n_1}\mathbf{M}_1, \dots, {}^{n_l}\mathbf{M}_l)$. If either the constitutive variable, here $\mathbf{C}$, or the tuple of structural tensors $\mathcal{M}_\mathcal{G}$ is transformed separately by any $\mathbf{Q} \in \mathcal{G}$, the conditions

$$\begin{aligned} &I(\mathbf{C}, \mathcal{M}_\mathcal{G}) = I(\mathbf{Q} \star \mathbf{C}, \mathcal{M}_\mathcal{G})\ \forall\, \mathbf{C} \in \mathcal{L}^2_{\mathrm{sym}}, \mathbf{Q} \in \mathcal{G} \subseteq \mathcal{O}(3) \quad \wedge \quad I(\mathbf{C}, \mathcal{M}_\mathcal{G}) \neq I(\mathbf{Q} \star \mathbf{C}, \mathcal{M}_\mathcal{G})\ \forall\, \mathbf{C} \in \mathcal{L}^2_{\mathrm{sym}}, \mathbf{Q} \notin \mathcal{G} \subseteq \mathcal{O}(3)\ , \\ &I(\mathbf{C}, \mathcal{M}_\mathcal{G}) = I(\mathbf{C}, \mathbf{Q} \star \mathcal{M}_\mathcal{G})\ \forall\, \mathbf{C} \in \mathcal{L}^2_{\mathrm{sym}}, \mathbf{Q} \in \mathcal{G} \subseteq \mathcal{O}(3) \quad \wedge \quad I(\mathbf{C}, \mathcal{M}_\mathcal{G}) \neq I(\mathbf{C}, \mathbf{Q} \star \mathcal{M}_\mathcal{G})\ \forall\, \mathbf{C} \in \mathcal{L}^2_{\mathrm{sym}}, \mathbf{Q} \notin \mathcal{G} \subseteq \mathcal{O}(3) \end{aligned} \tag{15}$$

follow, which again restrict the admissible transformations to the corresponding group $\mathcal{G}$.

2.4.3 Isotropic invariants of multiple tensors

Since we consider isotropic scalar-valued tensor functions, results on isotropic invariants from multiple tensors can be used directly. One of the most important works in this field is the one by Boehler (1977), which provides a functional basis (Def. 17), of isotropic homogeneous polynomial invariants, i.e., a functionally complete set of invariants (Def. 15). Thereby, the framework is valid for any number of 1st order tensors $\boldsymbol{v}_\alpha \in \mathcal{L}^1$, symmetric 2nd order tensors $\mathbf{A}_\beta \in \mathcal{L}^2_{\mathrm{sym}}$ and skew-symmetric 2nd order tensors $\mathbf{W}_\gamma \in \mathcal{L}^2_{\mathrm{skw}}$, cf. Tab. 13. To maintain consistency with the original work, we have chosen the same notation for the introduced tensors here. Since Boehler (1977) only considered scalar-valued invariants of 1st and 2nd order tensors, the tuple $\mathcal{M}_\mathcal{G}$ is naturally restricted to structural tensors of at most 2nd order when using the results from Tab. 13. Sect. 3.1 therefore introduces the approach by Xiao (1996a) to exchange the tuple $\mathcal{M}_\mathcal{G}$, enabling the results of Boehler (1977) to be applied also to cases involving structural tensors of 3rd or higher order. Thus, to this point, a functional basis can be obtained from the results of Boehler (1977) for all cases with 1st and 2nd order structural tensors.

Remark 2. An integrity basis is always also a functional basis, while the opposite does not hold in general. In many cases, however, the isotropic invariants of Boehler (1977) also represent an integrity basis. Alternatively, this is guaranteed with the invariants proposed by Smith (1965).

In general, according to Pennisi & Trovato (1987), the functional basis of Boehler (1977) is functionally irreducible. However, since Boehler's basis was formulated for non-constant arguments or tensors, polynomial relations between invariants arise here due to the constancy of structural tensors (Boehler, 1979). In turn, this implies that the functional or integrity basis for a specific anisotropy obtained from Tab. 13 does not yield a polynomially/functionally irreducible set of invariants (Apel, 2004, Ebbing, 2010). As a result, numerous works (Apel, 2004, Ebbing, 2010, Kalina et al., 2024a) are limited to invariants of lower polynomial degree in order to reduce the number of invariants in a material model.

Remark 3. Pennisi & Trovato (1987) showed that each invariant $I_\mu : \mathcal{H}_{\mathcal{O}(3)} \mapsto I_\mu\left(\mathcal{H}_{\mathcal{O}(3)}\right)$ defined by Boehler (1977) can not be represented as a function of the others, but more general algebraic dependencies between the invariants may be overlooked.[7] As an example, let $\mathcal{E} = \{I_1, I_2, \dots, I_K\}$, $K \in \mathbb{Z}_{\geq 1}$ be any set of invariants according to Boehler (1977). All considered invariants are then evaluated for two different states of the tensors in $\mathcal{H}_{\mathcal{O}(3)}$, which are chosen such that, for example, the invariants $\{I_1, I_2, \dots, I_{K-1}\}$ have the same value for both states, while I_K takes different values for the two states. From this, it was concluded that I_K can not be a function of the invariants $I_1, I_2, \dots, I_{K-1}$. However, it should be noted that this does not demonstrate algebraic independence of the invariants. If, for example, a homogeneous polynomial relation (syzygy) exists in the form $\sum_{\alpha=0}^{p} f_\alpha(I_1, I_2, \dots, I_{K-1}) I_K^\alpha = 0$, where f_α is a homogeneous polynomial and $p > 1$ denotes the number of terms, then I_K

[7] Originally, Pennisi & Trovato (1987) used the terminology single-valued function instead of function.

may be expressed as a multi-valued algebraic function of $I_1, I_2, \ldots, I_{K-1}$, i.e., the set of roots. Consequently, the method of Pennisi & Trovato (1987) may overlook certain cases of algebraic dependency between invariants, as illustrated by the example given in C.

3 Construction of irreducible integrity bases via structural tensors

In this section, we introduce a framework for identifying polynomially irreducible invariants from a polynomially complete set of invariants, i.e., an irreducible integrity basis. This is followed by two examples: the monoclinic anisotropy $\mathscr{A}_2$ and the cubic anisotropy $\mathscr{A}_{10}$.

3.1 Constructing complete invariant sets via Xiao's approach

The result of Boehler (1977) for constructing functional bases, presented in Tab. 13, is restricted to 1st and 2nd order tensors. However, since not all anisotropies can be represented by structural tensors that are of at most 2nd order (Xiao et al., 2006), the tuple $\mathcal{M}_{\mathcal{G}}$ of structural tensors was generalized by Xiao (1996a) to a tuple $\mathcal{F}_{\mathcal{G}}$ of structural functions

$$\mathcal{F}_{\mathcal{G}} = (\boldsymbol{v}_1(\mathbf{C}), \boldsymbol{v}_2(\mathbf{C}), .., \boldsymbol{v}_a(\mathbf{C}), \mathbf{A}_1(\mathbf{C}), \mathbf{A}_2(\mathbf{C}), .., \mathbf{A}_b(\mathbf{C}), \mathbf{W}_1(\mathbf{C}), \mathbf{W}_2(\mathbf{C}), .., \mathbf{W}_c(\mathbf{C})) \ , \ a, b, c \in \mathbb{Z}_{\geq 0} \ . \tag{16}$$

The arguments $\boldsymbol{v}_\alpha(\mathbf{C}) \in \mathcal{L}^1$, $\mathbf{A}_\beta(\mathbf{C}) \in \mathcal{L}^2_{\text{sym}}$ and $\mathbf{W}_\gamma(\mathbf{C}) \in \mathcal{L}^2_{\text{skw}}$ are now tensor functions depending on $\mathbf{C}$ and structural tensors ${}^n\mathbf{M} \in \mathcal{L}^n$ whose order can be greater than two. For simplicity, the functional dependence on the structural tensors ${}^n\mathbf{M}$ in Eq. (16) has been omitted. Hence, with Tab. 13 of Boehler (1977) and the tuple $\mathcal{F}_{\mathcal{G}}$, a functionally complete but not necessarily polynomially/functionally irreducible set of invariants can be obtained. It should be emphasized once again that the basis of Boehler (1977) does not guarantee the construction of an integrity basis, see Remark 2. However, in all cases examined in this work, an integrity basis can be obtained by combining suitable structural tensors in conjunction with the basis of Boehler (1977).

Remark 4. In the examined cases, it is sufficient to only consider structural functions up to the order of $\mathbf{C}^2$, cf. Kalina et al. (2024a). For example, structural tensor functions take the form ${}^4\mathbf{M} : \mathbf{C}$, ${}^4\mathbf{M} : \mathbf{C}^2$, ${}^4\mathbf{M} : \mathbf{C}^3$, where ${}^4\mathbf{M} \in \mathcal{L}^4$ denotes a constant 4th order structural tensor. By using the Cayley-Hamilton theorem,

$$\mathbf{C}^3 = I_1\mathbf{C}^2 - I_2\mathbf{C} + I_3\mathbf{1} \tag{17}$$

follows. When Eq. (17) is multiplied by ${}^4\mathbf{M}$, it becomes evident that structural functions ${}^4\mathbf{M} : \mathbf{C}^n$ up to at most second order ($n = 2$) are sufficient, as higher-order terms ($n > 2$) can be expressed in terms of lower-order terms ${}^4\mathbf{M} : \mathbf{C}^n, n \in \{0, 1, 2\}$ and the three well-known isotropic invariants

$$\mathrm{I}_1 = \mathrm{tr}[\mathbf{C}], \quad I_2 = \frac{1}{2}\left(\mathrm{tr}^2[\mathbf{C}] - \mathrm{tr}[\mathbf{C}^2]\right) \quad \text{and} \quad I_3 = \det[\mathbf{C}] \ , \tag{18}$$

with $\mathrm{tr}[\bullet]$ and $\det[\bullet]$ denoting the trace and determinant of the argument $\bullet$, respectively.

3.2 Elimination of reducible invariants

Let $\{{}^{n_1}I_1, {}^{n_2}I_2, \ldots, {}^{n_L}I_L\}$, $L \in \mathbb{Z}_{\geq 1}$ be a polynomially complete but reducible set of homogeneous polynomial invariants and $\mathcal{X}_{\mathcal{G}}$ a tuple of these invariants sorted in ascending order of polynomial degree $n_\nu \in \mathbb{Z}_{>0}$. In order to determine which invariants are polynomially reducible, it is necessary to identify the syzygies of the form

$${}^{n_\nu}I_\nu = f\left({}^{n_1}I_1, {}^{n_2}I_2, \ldots, {}^{n_{\nu-1}}I_{\nu-1}, {}^{n_{\nu+1}}I_{\nu+1}, \ldots, {}^{n_L}I_L\right) \ , \tag{19}$$

where $f \in \mathbb{R}_{\mathcal{G}}[x_1, \ldots, x_m]$ denotes a homogeneous polynomial in a finite number of invariants, which depend on the variables $x_1, \ldots, x_m$, and $\mathbb{R}_{\mathcal{G}}[x_1, \ldots, x_m]$ the ring of $\mathcal{G}$-invariant polynomails (Def. 8). Since identifying polynomial relationships between invariants can become arbitrarily complex, we present a general framework for efficiently determining such relationships using an analytical-numerical approach in the following.

3.2.1 General approach

As a first step, we outline the principles behind constructing a polynomially complete and irreducible invariant set $\mathcal{J}_{\mathcal{G}}$, i.e., an irreducible integrity basis, from a polynomially complete but possibly reducible invariant set from the tuple $\mathcal{X}_{\mathcal{G}} = ({}^{n_1}I_1, {}^{n_2}I_2, \ldots, {}^{n_L}I_L)$. Initially, the invariant ${}^{n_1}I_1$ with $n_1 \in \mathbb{Z}_{\geq 0}$ is selected as an element ${}^{n_1}\tilde{I}_1 = {}^{n_1}I_1$ of the preliminary tuple $\mathcal{Y}_{\mathcal{G}} = \left({}^{n_1}\tilde{I}_1\right)$ of polynomially irreducible invariants. Subsequently, the next invariant ${}^{n_2}I_2$ from the tuple $\mathcal{X}_{\mathcal{G}}$ is considered, and a complete polynomial ansatz ${}^{n_2}I_2 = f\left({}^{n_1}\tilde{I}_1\right)$ is made to express it as a polynomial in the invariants of $\mathcal{Y}_{\mathcal{G}}$, where each summand of $f\left({}^{n_1}\tilde{I}_1\right)$ has degree n_2. If ${}^{n_2}I_2$ can be represented as a polynomial in the invariants of $\mathcal{Y}_{\mathcal{G}}$, the invariant is considered trivial and the procedure is repeated for the next invariant ${}^{n_3}I_3$ in $\mathcal{X}_{\mathcal{G}}$. Otherwise, ${}^{n_2}\tilde{I}_2 = {}^{n_2}I_2$ is added to tuple $\mathcal{Y}_{\mathcal{G}}$, and the polynomial ansatz is extended accordingly for the remaining invariants. By applying this procedure to all remaining invariants, a polynomially complete and irreducible set $\mathcal{J}_{\mathcal{G}}$ of invariants is obtained, whose elements are the elements of the final tuple $\mathcal{Y}_{\mathcal{G}}$.

3.2.2 Analytical-numerical approach

While the overall procedure in Sect. 3.2.1 is well understood, the primary challenge lies in identifying the polynomial relationships (19), or to be more precise, the coefficients of the complete polynomial ansatz. Therefore, we present below an efficient method for determining the unknown coefficients for each invariant ${}^{n_\mu}I_\mu$ out of $\mathcal{X}_\mathcal{G}$. For the μth invariant we start with a numerical step as an initial guess, which is followed by an analytical step using symbolic computations.

Numerical step for the μth invariant Within this paragraph, we do not use the summation convention. First, for a given point group or anisotropy, the tuple $\mathcal{X}_\mathcal{G}$ of L invariants, forming a polynomially complete set, is assembled based on the corresponding tuple $\mathcal{F}_\mathcal{G}$ of structural functions and by using Tab. 13 of Boehler (1977). Subsequently, the invariants

$$
{}^{n_\mu}I_{\mu,\Lambda} = {}^{n_\mu}I_\mu\left(\mathbf{C}_\Lambda\right) \ , \ \mu \in \{1, 2, \dots, L\} \tag{20}
$$

are evaluated for multiple randomly generated instances of the tensor $\mathbf{C}$, where we use $\Lambda \in \{1, 2, \dots, N\}$ for labeling. The coordinates of these instances are drawn from a normal distribution with a mean of 0 and a standard deviation of 1, where symmetry of $\mathbf{C}$ is ensured but not positive definiteness.[8] Hence, ${}^{n_\mu}I_{\mu,\Lambda} \in \mathbb{R}$ represents a vector ${}^{n_\mu}\underline{\boldsymbol{I}}_\mu \in \mathbb{R}^{N\times 1}$. According to their prescribed formation rules, the structural tensors are computed for a random orientation that is hold constant for all instances Λ. Then, a complete polynomial ansatz for the μth invariant from $\mathcal{X}_\mathcal{G}$ is made:

$$
{}^{n_\mu}I_{\mu,\Lambda} = \sum_{\alpha=1}^{P} {}^{n_\mu}J_{\mu,\Lambda\alpha}a_{\mu,\alpha} \quad \text{for all states } \Lambda \quad \leftrightarrow \quad {}^{n_\mu}\underline{\boldsymbol{I}}_\mu = {}^{n_\mu}\underline{\underline{\boldsymbol{J}}}_\mu \cdot \underline{\boldsymbol{a}}_\mu \ . \tag{21}
$$

Thereby, $J_{\mu,\Lambda\alpha} \in \mathbb{R}$ represent the coefficients of a matrix ${}^{n_\mu}\underline{\underline{\boldsymbol{J}}}_\mu \in \mathbb{R}^{N\times P}$, with P denoting the number of terms in the ansatz, and $\underline{\boldsymbol{a}}_\mu \in \mathbb{R}^{P\times 1}$ a vector of unknown coefficients $a_{\mu,\alpha} \in \mathbb{R}$. Each column of the matrix represents an argument in the ansatz, i.e., an invariant

$$
{}^{n_\mu}J_{\mu,\Lambda\alpha} = \prod_{\nu\in\mathcal{A}_{\mu,\alpha}} {}^{n_\nu}\tilde{I}_\nu(\mathbf{C}_\Lambda) \ , \ {}^{n_\nu}\tilde{I}_\nu \in \mathcal{Y}_\mathcal{G} \quad \text{with} \quad \sum_{\nu\in\mathcal{A}_{\mu,\alpha}} n_\nu = n_\mu \ , \tag{22}
$$

that is constructed from a (sub)tuple of the irreducible invariants ${}^{n_\nu}\tilde{I}_\nu$ within the current $\mathcal{Y}_\mathcal{G}$ for all instances Λ. Thereby, the tuple $\mathcal{A}_{\mu,\alpha}$ contains the indices $\nu \in \mathcal{A}_{\mu,\alpha}$ such that the polynomial degree of the product in the polynomially irreducible invariants ${}^{n_\nu}\tilde{I}_\nu$ equals the degree n_μ of the μth invariant from $\mathcal{X}_\mathcal{G}$. Since multiplication is commutative, it follows from Eq. (22) that of all possible tuples $\mathcal{A}_{\mu,\alpha}$ only one realization of a every allowed permutation is required. Hence, the index α goes from 1 to the number of different allowed permutations P.

To determine the coefficients $\underline{\boldsymbol{a}}_\mu$ for the μth invariant, we formulate the linear optimization problem

$$
\underline{\hat{\boldsymbol{a}}}_\mu = \underset{\underline{\boldsymbol{a}}_\mu\in\mathbb{R}^{P\times 1}}{\arg\min} \left| {}^{n_\mu}\underline{\boldsymbol{I}}_\mu - {}^{n_\mu}\underline{\underline{\boldsymbol{J}}}_\mu \cdot \underline{\boldsymbol{a}}_\mu \right|^2 \tag{23}
$$

that yields the necessary condition $({}^{n_\mu}\underline{\underline{\boldsymbol{J}}}_\mu)^\top \cdot \left[{}^{n_\mu}\underline{\boldsymbol{I}}_\mu - {}^{n_\mu}\underline{\underline{\boldsymbol{J}}}_\mu \cdot \underline{\boldsymbol{a}}_\mu \right] = \underline{\boldsymbol{0}}$. We solve the problem given above by using NumPy's least squares method. If all entries

$$
\left({}^{n_\mu}J_{\mu,\Lambda 1}, {}^{n_\mu}J_{\mu,\Lambda 2}, \dots, {}^{n_\mu}J_{\mu,\Lambda\alpha}, \dots, {}^{n_\mu}J_{\mu,\Lambda P}\right) \tag{24}
$$

obtained from Eq. (22) are linear independent, it follows that the determined coefficients $\hat{a}_{\mu,\alpha}$ of the linear optimization task are unique. After solving the problem (23), the norm

$$
R_\mu = \max_\Lambda \left| \sum_{\alpha=1}^{P} \hat{a}_{\mu,\alpha} {}^{n_\mu}J_{\mu,\Lambda\alpha} - {}^{n_\mu}I_{\mu,\Lambda} \right| \rightarrow \begin{array}{ll} R_\mu < \text{tol} \rightarrow & \text{trivial invariant} \\ R_\mu \geq \text{tol} \rightarrow & \text{irreducible invariant} \end{array} \tag{25}
$$

is employed to verify whether the given invariant can be accurately represented as a polynomial, with $\max\limits_\Lambda|\bullet|$ denoting the Chebyshev distance. In the cases studied, a number of 1000 randomly generated states and a tolerance value tol = 1 were found to yield reliable results in a couple of seconds. If it turns out that the μth invariant is reducible and the exact coefficients of the found relation are of interest, the analytical step is carried out. Otherwise, ${}^{n_{\kappa+1}}\tilde{I}_{\kappa+1} = {}^{n_\mu}I_\mu$ is added to the current tuple $\mathcal{Y}_\mathcal{G}$ with κ elements and the numerical step is directly executed again for the next invariant ${}^{n_{\mu+1}}I_{\mu+1}$ in $\mathcal{X}_\mathcal{G}$.

[8]Positive definiteness does not affect the algorithm, as the invariants of Boehler (1977) are not subject to this constraint either.

Analytical step for the μth invariant The syzygies found numerically are initially very good approximations, which are then verified symbolically in a subsequent step. For this purpose, we use the SymPy library, which provides the invariants in analytical form. For every found syzygy, the verification process begins by examining the solution vector $\underline{\hat{\boldsymbol{a}}}_\mu$ to determine whether the coefficients $\hat{a}_{\mu,\alpha}$ can be expressed as rational numbers. If this is the case, the identified syzygy between the invariants is checked for exactness.

Remark 5. In general, the number of random states must be greater than or equal to the number of terms in the polynomial ansatz. When the ansatz involves high polynomial degrees, numerical errors may accumulate, potentially leading to incorrect identification of invariants as either reducible or irreducible. This issue can be mitigated by increasing the precision of floating-point values or by switching to symbolic computation also for the numerical step. However, this comes at the cost of increased computational time. Thus, fully symbolic computation should be avoided if possible and only used to perform the analytical step.

Remark 6. The presented procedure serves not only to derive an irreducible integrity basis from a polynomially complete set of invariants, but also to identify algebraic relations in higher polynomial degrees between polynomially irreducible invariants. Furthermore, polynomial syzygies between distinct sets of invariants are also obtainable with this numerical-analytical approach.

3.3 Proof of completeness and irreducibility

In the following, we present two approaches to verify polynomial completeness and irreducibility of a set of invariants: one based on the Molien series, and another involving a comparison with an already established set of polynomially complete and irreducible invariants in coordinate-dependent form.

3.3.1 Molien series

The Hilbert series, which is often converted into the Molien series (MS) using Molien's theorem, provides important information about the number of invariants in each polynomial degree that are required for a polynomially complete and irreducible set of invariants (Derksen & Kemper, 2002, Sturmfels, 2008).[9] The MS can be calculated by

$$\mathscr{M}_{\mathcal{G}} = \frac{1}{|\mathcal{G}|} \sum_{\mathbf{Q} \in \mathcal{G}} \frac{1}{\det\left(\underline{\underline{\mathbf{1}}} - t\underline{\underline{\boldsymbol{\Phi}}}\left(\mathbf{Q}\right)\right)} \,, \tag{26}$$

where $\underline{\underline{\mathbf{1}}} \in \mathbb{R}^{n\times n}$ denotes the n-dimensional identity matrix, $t \in (-1, 1)$ a parameter and $\underline{\underline{\boldsymbol{\Phi}}} \in \mathbb{R}^{n\times n}$ a transformation matrix depending on a group element $\mathbf{Q} \in \mathcal{G}$. In the present context of hyperelasticity $n = 6$.

For identifying the coefficients $\Phi_{\alpha\beta} \in \mathbb{R}$ of $\underline{\underline{\boldsymbol{\Phi}}} \in \mathbb{R}^{6\times 6}$, we begin by referring to Eq. (3), where the symmetric tensor $\mathbf{C} \in \mathcal{L}^2_{\text{sym}}$ is transformed by an element $\mathbf{Q} \in \mathcal{O}(3)$. However, since we are now interested in material symmetry, we will only consider $\mathbf{Q} \in \mathcal{G} \subseteq \mathcal{O}(3)$. Instead of performing this transformation directly in $\mathcal{L}^2_{\text{sym}}$, it can alternatively be carried out by transforming the tensor in vector notation $\underline{\boldsymbol{C}} \in \mathbb{R}^{6\times 1}$ with a transformation matrix $\underline{\underline{\boldsymbol{\Phi}}}$. For this purpose, the relationships

$$C_\alpha = T^\alpha_{ij} C_{ij} \quad \text{and} \quad C_{ij} = \tilde{T}^{ij}_\alpha C_\alpha \tag{27}$$

should hold between the tensor coordinates C_{ij} and the vector coordinates C_α, where T^α_{ij} and $\tilde{T}^{ij}_\alpha$ are suitable transformation coefficients. We note that

$$T^\alpha_{ij} \tilde{T}^{ij}_\beta = \delta_{\alpha\beta} \quad \text{and} \quad T^\alpha_{ij} \tilde{T}^{kl}_\alpha = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) \tag{28}$$

have to be true. By imposing $T^\alpha_{ij} = \tilde{T}^{ij}_\alpha$, Eq. (27) becomes

$$C_\alpha = T^\alpha_{ij} C_{ij} \quad \text{and} \quad C_{ij} = T^\alpha_{ij} C_\alpha \tag{29}$$

and the product

$$\mathbf{C} : \mathbf{C} = \underline{\boldsymbol{C}} \cdot \underline{\boldsymbol{C}} \quad \leftrightarrow \quad C_{ij}C_{ji} = C_\alpha C_\alpha \tag{30}$$

is equal in both spaces. The transformation coefficients

$$T^\alpha_{ij} = \begin{cases} 1 & \alpha = i = j \\ \frac{1}{\sqrt{2}} & (\alpha, i, j) = \{(4,2,3), (4,3,2), (5,1,3), (5,3,1), (6,1,2), (6,2,1)\} \\ 0 & \text{else} \end{cases} \tag{31}$$

[9] In some works in literature (Derksen & Kemper, 2002, Neusel, 2007, Teranishi, 1986), the Hilbert series is also referred to as Poincaré series.

fulfill the relations in Eq. (29). Hence, the resulting vector $\underline{\boldsymbol{C}}$ corresponds to the Kelvin-Mandel notation of the tensor $\mathbf{C}$ (Brannon, 2018). In this representation, $\mathbf{Q} \star \mathbf{C}$ is represented by $\underline{\underline{\boldsymbol{\Phi}}} \cdot \underline{\boldsymbol{C}}$, where $\underline{\underline{\boldsymbol{\Phi}}}$ is the 6×6 rotation matrix in Kelvin-Mandel notation, whose coefficients $\Phi_{\alpha\beta}$ can be computed using

$$\Phi_{\alpha\beta} = T^{\alpha}_{ik} T^{\beta}_{jl} Q_{ij} Q_{kl} \quad , \quad \mathbf{Q} \in \mathcal{G} \, . \tag{32}$$

Thus, the full matrix $\underline{\underline{\boldsymbol{\Phi}}}$ is denoted by

$$\left[\Phi_{\alpha\beta}\right] = \begin{pmatrix} Q_{11}^2 & Q_{12}^2 & Q_{13}^2 & \sqrt{2}Q_{12}Q_{13} & \sqrt{2}Q_{11}Q_{13} & \sqrt{2}Q_{11}Q_{12} \\ Q_{21}^2 & Q_{22}^2 & Q_{23}^2 & \sqrt{2}Q_{22}Q_{23} & \sqrt{2}Q_{21}Q_{23} & \sqrt{2}Q_{21}Q_{22} \\ Q_{31}^2 & Q_{32}^2 & Q_{33}^2 & \sqrt{2}Q_{32}Q_{33} & \sqrt{2}Q_{31}Q_{33} & \sqrt{2}Q_{31}Q_{32} \\ \sqrt{2}Q_{21}Q_{31} & \sqrt{2}Q_{22}Q_{32} & \sqrt{2}Q_{23}Q_{33} & Q_{22}Q_{33}+Q_{23}Q_{32} & Q_{21}Q_{33}+Q_{23}Q_{31} & Q_{21}Q_{32}+Q_{22}Q_{31} \\ \sqrt{2}Q_{11}Q_{31} & \sqrt{2}Q_{12}Q_{32} & \sqrt{2}Q_{13}Q_{33} & Q_{12}Q_{33}+Q_{13}Q_{32} & Q_{11}Q_{33}+Q_{13}Q_{31} & Q_{11}Q_{32}+Q_{12}Q_{31} \\ \sqrt{2}Q_{11}Q_{21} & \sqrt{2}Q_{12}Q_{22} & \sqrt{2}Q_{13}Q_{23} & Q_{12}Q_{23}+Q_{13}Q_{22} & Q_{11}Q_{23}+Q_{13}Q_{21} & Q_{11}Q_{22}+Q_{12}Q_{21} \end{pmatrix} . \tag{33}$$

From Eq. (32) and the transformation coefficients T^{α}_{ij}, it follows directly that the matrix $\underline{\underline{\boldsymbol{\Phi}}}$ is diagonal if the transformation $\mathbf{Q} \in \mathcal{G}$ lies in the principle-axis state. Furthermore, for any $\mathbf{Q} = \pm\mathbf{Q}^{\varphi}_{\boldsymbol{a}} \in \mathcal{G} \subseteq \mathcal{O}(3)$, the eigenvalues of $\pm\mathbf{Q}^{\varphi}_{\boldsymbol{a}}$ are denoted by $\left\{\pm 1, \pm e^{i\varphi}, \pm e^{-i\varphi}\right\}$ for an arbitrary rotation angle $\varphi \in [0, 2\pi)$. Finally, this allows us to express the determinant

$$\det\left(\underline{\underline{\mathbf{1}}} - t\underline{\underline{\boldsymbol{\Phi}}}(\mathbf{Q})\right) = f(\varphi) = (1-t)^2(1 - 2t\cos(\varphi) + t^2)(1 - 2t\cos(2\varphi) + t^2) \tag{34}$$

in Eq. (26) as a function of the rotation angle of a group element.[10] If the MS is formed according to Eq. (26) and converted into a form

$$\mathcal{M}_{\mathcal{G}} = \frac{1 + a_1 t + a_2 t^2 + \cdots + a_{s-1}t^{s-1} + a_s t^s}{(1-t)^{p_1}\left(1-t^2\right)^{p_2} \ldots \left(1-t^{n-1}\right)^{p_{n-1}} (1-t^n)^{p_n}} \quad \text{with} \quad a_\lambda, p_\mu, s \in \mathbb{Z}_{\geq 0} \quad \text{and} \quad \lambda, \mu, n \in \mathbb{Z}_{>0} \, , \tag{35}$$

then several information can be extracted. The factors of the denominator provide information about the number p_μ and polynomial degree μ of the primary invariants (Def. 12), while the coefficients a_λ of the numerator indicate how many secondary invariants (Def. 13) exist in the corresponding polynomial degree λ (Sturmfels, 2008). Another representation of the MS is the corresponding Taylor series

$$\mathcal{M}_{\mathrm{Tay},\mathcal{G}} = \sum_{i=1}^{\infty} \frac{1}{i!} \left.\frac{\mathrm{d}^i \mathcal{M}(t)}{\mathrm{d}t^i}\right|_{t=0} = 1 + b_1 t + b_2 t^2 + b_3 t^3 + \mathrm{HOT}, \quad b_\lambda \in \mathbb{Z}_{\geq 0} \, , \tag{36}$$

where HOT denotes higher order terms. The coefficients b_λ indicate the number of all independent invariants of polynomial degree λ, i.e., all fundamental invariants as well as the independent invariants that can be formed trivially from invariants of lower polynomial degree (Sturmfels, 2008). Combinatorial reasoning then allows to determine the number of fundamental invariants as well as syzygies between them from the coefficients b_i (Sturmfels, 2008), which is illustrated in Sects. 3.4 and 3.5. However, when both fundamental invariants as well as syzygies appear at the same degree, the separation between them becomes ambiguous.

Therefore, the MS is a powerful tool for counting invariants and provides an efficient method of assessing whether a given set of invariants is polynomially complete and irreducible.

Remark 7. A set of primary (Def. 12) and secondary (Def. 13) invariants does not have to be polynomially irreducible, because some secondary invariants may be products of other secondary invariants (Smith, 1962). An irreducible integrity basis, on the other hand, only contains the fundamental invariants (Def. 11), that are the primary and polynomially irreducible secondary invariants. In order to prove polynomial completeness and irreducibility with the information provided by the MS, it is therefore usually necessary to find the syzygies between the invariants.

Remark 8. The number of primary invariants is equal to the number of independent tensor coordinates for any finite group that is a subgroup of the general linear group (Sturmfels, 2008). Thus, for any finite group $\mathcal{G} \subseteq \mathcal{O}(3)$ and a given tensor $\mathbf{C} \in \mathcal{L}^2_{\mathrm{sym}}$, the number of primary invariants is always six. This fact allows for a validation of the MS as expressed in Eq. (35).

[10]For any even-order tensor, which is not a two-point tensor, transformations with $+\mathbf{Q}^{\varphi}_{\boldsymbol{a}}$ and $-\mathbf{Q}^{\varphi}_{\boldsymbol{a}}$ are identical, see Remark 1. This equivalence is also reflected in the fact that the expressions of the determinant for both $+\mathbf{Q}^{\varphi}_{\boldsymbol{a}}$ and $-\mathbf{Q}^{\varphi}_{\boldsymbol{a}}$ yield the same result. In contrast, for odd-order tensors, the transformation behavior differs, resulting in two distinct formula for $+\mathbf{Q}^{\varphi}_{\boldsymbol{a}}$ and $-\mathbf{Q}^{\varphi}_{\boldsymbol{a}}$.

3.3.2 Usage of a known irreducible integrity basis

Instead of relying on the MS to demonstrate polynomial completeness and irreducibility, one can alternatively prove this by identifying the polynomial syzygies to another known irreducible integrity basis like that from Smith (1962), which is constituted by invariants in coordinate-dependent form. The syzygies can be obtained in a straight forward manner with the algorithm introduced in Sect. 3.2. In the following, we present a more formal discussion to support this claim.

Proposition 1. Let $\mathcal{G}$ be a group, $r, q \in \mathbb{Z}_{>0}$ and let $\{I_1, \dots, I_r\}$ a functionally complete set of scalar-valued $\mathcal{G}$-invariants. Furthermore, let $\left\{J_1, \dots, J_q\right\}$ another set of scalar $\mathcal{G}$-invariants such that for all $\alpha \in \{1, \dots, r\}$, the invariants of the first set can be expressed as a function of the form $I_\alpha = \bar{I}_\alpha(J_1, \dots, J_q)$. Then $\left\{J_1, \dots, J_q\right\}$ is also functionally complete.

Proof. As $\{I_1, \dots, I_r\}$ is functionally complete, for every scalar-valued $\mathcal{G}$-invariant Z there exists a function $f(I_1, \dots, I_r)$ such that $Z = f(I_1, \dots, I_r)$. Inserting $I_\alpha = \bar{I}_\alpha(J_1, \dots, J_q)$ for $\alpha \in \{1, \dots, r\}$, we obtain

$$Z = f(I_1(J_1, \dots, J_q), \dots, I_r(J_1, \dots, J_q)) = g(J_1, \dots, J_q)\ .$$

Thus, Z can also be written as function g of the elements of $\left\{J_1, \dots, J_q\right\}$, which therefore is functionally complete. □

Note that similar arguments can be used to show polynomial completeness, i.e., to prove that an invariant set is an integrity basis.

Lemma 2. Let $k, m, n \in \mathbb{Z}_{>0}$ and $F \in \mathbb{R}[x_1, \dots, x_n]$ be a polynomial in the variables $x_1, \dots, x_n$. Furthermore, let $P_1, \dots, P_n \in \mathbb{R}[y_1, \dots, y_m]$ be homogeneous polynomials in the variables $y_1, \dots, y_m$. Consider $F(P_1, \dots, P_n) \in \mathbb{R}[y_1, \dots, y_m]$ and let $\deg(F(P_1, \dots, P_n)) = q$. Let $\deg(P_i) \le q\ \forall i \in \{1, \dots, k\}$ and $\deg(P_i) > q\ \forall i \in \{k+1, \dots, n\}$. Then there is a polynomial $G \in \mathbb{R}[x_1, \dots, x_k]$ such that $G(P_1, \dots, P_k) = F(P_1, \dots, P_k, \dots, P_n)$.

Proof. F can be described as a linear combination of monomials. Consequently, $F(P_1, \dots, P_n)$ is a sum of elements of the form $\lambda P_1^{\epsilon_1} \dots P_n^{\epsilon_n}$, where $\lambda \in \mathbb{R}$ and $\epsilon_i \in \mathbb{Z}_{\ge 0}$. Since all P_i are homogeneous polynomials, these elements are homogeneous polynomials of degree $\epsilon_1 \deg(P_1) + \dots + \epsilon_n \deg(P_n)$. One can split F into $F = G + H$, where G denotes the sum of all the monomials $M = x_1^{\epsilon_1} \dots x_n^{\epsilon_n}$ of F with $\epsilon_1 \deg(P_1) + \dots + \epsilon_n \deg(P_n) \le q$ and H the remaining monomials. Since $F(P_1, \dots, P_n)$ has degree q, and since $H(P_1, \dots, P_n)$ is a sum of monomials of degree no less than $q+1$, then $H(P_1, \dots, P_n) = 0$, implying $F(P_1, \dots, P_n) = G(P_1, \dots, P_n)$. Furthermore, since $\deg(P_i) > q$ for $i > k$, all the monomials of G have $\epsilon_i = 0$ for $i > k$. Consequently, G is only dependent on $P_1, \dots, P_k$ and the previous equality can be written as $F(P_1, \dots, P_n) = G(P_1, \dots, P_k)$. □

Proposition 3. Let $\mathcal{G}$ be a group, $a, n \in \mathbb{Z}_{>0}$ and $\mathbb{R}_\mathcal{G}[x_1, \dots, x_n] \subset \mathbb{R}[x_1, \dots, x_n]$ the ring of $\mathcal{G}$-invariant polynomials in the variables $x_1, \dots, x_n$. Furthermore, let $\{I_1, \dots, I_a\} \subset \mathbb{R}_\mathcal{G}[x_1, \dots, x_n]$ be a polynomially complete set of homogeneous irreducible polynomials. Let $\{J_1, \dots, J_a\} \subset \mathbb{R}_\mathcal{G}[x_1, \dots, x_n]$ be another polynomially complete set of homogeneous $\mathcal{G}$-invariant polynomials, with $\deg I_\ell = \deg J_\ell\ \forall\, \ell \in \{1, \dots, a\}$. Then $\{J_1, \dots, J_a\}$ is also polynomially irreducible.

Proof. For a contradiction, assume that $\{J_1, \dots, J_a\}$ is polynomially reducible, i.e., there is an $i \in \{1, \dots, a\}$ such that there exists a polynomial $f \in \mathbb{R}[y_1, \dots, y_{i-1}, y_{i+1}, \dots, y_a]$ with $J_i = f(J_1, \dots, J_{i-1}, J_{i+1}, \dots, J_a)$. Let us admit (if necessary by permuting the indices) that $\deg(J_k) < q$ for $k < i$, $\deg(J_k) = q$ for $i \le k \le i+u$ and $\deg(J_k) > q$ for $k > i+u$. Consider $\mathcal{R}_q \subseteq \mathbb{R}_\mathcal{G}[x_1, \dots, x_n]$ to be the set of invariant homogeneous polynomials of degree q. Remark that $\mathcal{R}_q$ naturally holds an $\mathbb{R}$-vector space structure with the standard addition and multiplication by a scalar. For $P \in \mathcal{R}_q$, there exists a polynomial F with $P = F(J_1, \dots, J_a)$. Since P has degree q and from Lemma 2, there exists a polynomial G with $P = G(J_1, \dots, J_{i+u})$. Since all monomials of P should have degree q,

$$P = \sum_{k=i}^{i+u} \lambda_k J_k + \widehat{G}(J_1, \dots, J_{i-1}) \qquad \text{with } \widehat{G}(J_1, \dots, J_{i-1}) \in \mathcal{R}_q$$

Particularly, this applies to J_i, and our assumption is equivalent to an equation of the form:

$$0 = -J_i + \sum_{k=i+1}^{i+u} \lambda_k J_k + \widehat{G}(J_1, \dots, J_{i-1}) \qquad \text{with } \widehat{G}(J_1, \dots, J_{i-1}) \in \mathcal{R}_q$$

Let $Q_J = \{P(J_1, \dots, J_{i-1}) \mid P \text{ polynomial}\} \cap \mathcal{R}_q$. Remark that Q_J also naturally holds a vector space structure and is a subspace of $\mathcal{R}_q$. Thus, each element of the quotient vector space $\mathcal{R}_q / Q_J$ has the form $\sum_{k=1}^{i+u} \lambda_k J_k$, implying that $\{J_i, \dots, J_{i+u}\}$ is spanning $\mathcal{R}_q / Q_J$. Analogously, one can create the space $\mathcal{R}_q / Q_I$ spanned by $\{I_i, \dots, I_{i+u}\}$. Consider $P(J_1, \dots, J_{i-1}) \in Q_J$ for any polynomial P. For each $k \in \{1, \dots, i-1\}$, there exists a polynomial F_k with $F_k(I_1, \dots, I_a) = J_k$. By Lemma 2, it even reduces to a polynomial G_k with $G_k(I_1, \dots, I_{i-1}) = J_k$. Consequently:

$$P(J_1, \dots, J_{i-1}) = P(G_1(I_1, \dots, I_{i-1}), \dots, G_{i-1}(I_1, \dots, I_{i-1})) \in Q_I$$

This implies that $Q_J \subseteq Q_I$ and by symmetry of I_k and J_k, we conclude that $Q_J = Q_I =: Q$. Thus, $\{J_i, \ldots, J_{i+u}\}$ and $\{I_i, \ldots, I_{i+u}\}$ are two spanning sets of the same vector space $\mathcal{R}_q/Q$. But since $\{I_1, \ldots, I_a\}$ is irreducible, an equation of the form

$$0 = \sum_{k=i}^{i+u} \lambda_k I_k + G(I_1, \ldots, I_{i-1}) \qquad \text{with } G(J_1, \ldots, J_{i-1}) \in \mathcal{R}_q$$

is impossible. It implies that $\{I_i, \ldots, I_{i+u}\}$ is linearly independent in $\mathcal{R}_q/Q$ and forms a basis. Since $\{J_i, \ldots, J_{i+u}\}$ is a spanning set with the same number of elements as a basis, it also is a basis. Therefore, an equation of the form

$$0 = \sum_{k=i}^{i+u} \lambda_k J_k + G(J_1, \ldots, J_{i-1}) \qquad \text{with } G(J_1, \ldots, J_{i-1}) \in \mathcal{R}_q$$

is impossible, what is a contradiction to our starting assumption. □

3.4 Example: Monoclinic crystal system

The monoclinic crystal system comprises the point groups C_2, C_{1h} and C_{2h} leading to the same anisotropy $\mathscr{A}_2$ and equivalent integrity basis in hyperelasticity. We investigate how to determine an irreducible integrity basis.

Structural tensors and reducible integrity basis Since the integrity bases are equivalent for the tensor $\mathbf{C} \in \mathcal{L}^2_{\text{sym}}$ and C_2, C_{1h} and C_{2h}, we only consider the latter here. The corresponding structural tensors $\mathbf{P}_2 \in \mathcal{L}^2_{\text{sym}}$ and $\mathbf{G}_1 \in \mathcal{L}^2_{\text{skw}}$, introduced by Zheng & Spencer (1993), are denoted by

$$\mathbf{P}_2 = \boldsymbol{a}_1\boldsymbol{a}_1 - \boldsymbol{a}_2\boldsymbol{a}_2 \quad \text{and} \quad \mathbf{G}_1 = {}^3\mathbf{E} \cdot \boldsymbol{a}_3 = \boldsymbol{a}_1\boldsymbol{a}_2 - \boldsymbol{a}_2\boldsymbol{a}_1 \;, \tag{37}$$

where ${}^3\mathbf{E} \in \mathcal{L}^3_{\text{skw}}$ is the permutation tensor (or ${}^3\mathbf{E}$-Pseudotensor) and $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{a}_3 \in \mathcal{L}^1$ orthonormal 1st order tensors. To be able to determine a polynomially complete set of invariants with the table of Boehler (1977), we define the tuple of structural functions by

$$\mathcal{F}_{C_{2h}} = \mathcal{M}_{C_{2h}} = (\mathbf{P}_2, \mathbf{G}_1) \tag{38}$$

and the tuple of argument tensors by

$$\mathcal{H}_{C_{2h}} = (\mathbf{C}, \mathbf{P}_2, \mathbf{G}_1) \;. \tag{39}$$

Thus, the polynomially complete set of 14 invariants

$$\begin{aligned} &\operatorname{tr}[\mathbf{C}],\ \operatorname{tr}[\mathbf{C}^2],\ \operatorname{tr}[\mathbf{C}^3],\ \operatorname{tr}[\mathbf{C}\cdot\mathbf{P}_2],\ \operatorname{tr}[\mathbf{C}^2\cdot\mathbf{P}_2],\ \operatorname{tr}[\mathbf{C}\cdot\mathbf{P}_2^2],\ \operatorname{tr}[\mathbf{C}^2\cdot\mathbf{P}_2^2],\ \operatorname{tr}[\mathbf{C}\cdot\mathbf{G}_1^2],\ \operatorname{tr}[\mathbf{C}^2\cdot\mathbf{G}_1^2],\\ &\operatorname{tr}[\mathbf{C}^2\cdot\mathbf{G}_1^2\cdot\mathbf{C}\cdot\mathbf{G}_1],\ \operatorname{tr}[\mathbf{C}\cdot\mathbf{P}_2\cdot\mathbf{G}_1],\ \operatorname{tr}[\mathbf{C}^2\cdot\mathbf{P}_2\cdot\mathbf{G}_1],\ \operatorname{tr}[\mathbf{C}\cdot\mathbf{P}_2^2\cdot\mathbf{G}_1],\ \operatorname{tr}[\mathbf{C}\cdot\mathbf{G}_1^2\cdot\mathbf{P}_2\cdot\mathbf{G}_1] \end{aligned} \tag{40}$$

is obtained from Tab. 13 of Boehler (1977), excluding invariants that consist solely of structural tensors, since these are merely constants. Note that Boehler's method generates functional bases. However, as will be shown, here we also obtain an integrity basis, cf. Remark 2.

Irreducible integrity basis By applying the procedure outlined in Sect. 3.2 for eliminating polynomially reducible invariants, we obtain the irreducible integrity basis in Tab. 3 for group C_{2h} from the polynomially complete set of invariants in Eq. (40). As a proof of polynomial completeness and irreducibility, we utilize Proposition 3 by calculating the polynomial relations between the invariants from Tab. 3 and those proposed by Smith (1962). These are determined using again the procedure described in Sect. 3.2. To achieve this, the orientation of the structural tensors must be aligned with that of Smith's invariants, which is why $[\boldsymbol{a}_1] = (0, 1, 0)^\top$, $[\boldsymbol{a}_2] = (0, 0, 1)^\top$ and $[\boldsymbol{a}_3] = (1, 0, 0)^\top$ are set accordingly. The polynomial relationships between the two invariant sets are presented in Tab. 23 and the comparison of the polynomial degrees between both sets in Tab. 39.

Table 3: Irreducible integrity bases for C_{2h} and a tensor $\mathbf{C} \in \mathcal{L}^2_{\text{sym}}$ with the structural tensors $\mathbf{P}_2$ and $\mathbf{G}_1$ of Eq. (37).

$I_1 = \operatorname{tr}[\mathbf{C}]$	$I_2 = \operatorname{tr}[\mathbf{C}\cdot\mathbf{G}_1^2]$	$I_3 = \operatorname{tr}[\mathbf{C}\cdot\mathbf{P}_2]$	$I_4 = \operatorname{tr}[\mathbf{C}\cdot\mathbf{P}_2\cdot\mathbf{G}_1]$	$I_5 = \operatorname{tr}[\mathbf{C}^2]$	$I_6 = \operatorname{tr}[\mathbf{C}^2\cdot\mathbf{P}_2]$	$I_7 = \operatorname{tr}[\mathbf{C}^2\cdot\mathbf{P}_2\cdot\mathbf{G}_1]$

Molien series The groups C_2, C_{1h} and C_{2h} lead to the same MS in the present case, which is why the MS only has to be computed for one of the three. We show the calculation using C_2. This group is generated by $\mathbf{Q}_z^\pi$ and contains two group elements that hold one angle of π and one angle of 0, respectively. Hence, with Eqs. (26) and (34), the MS

$$\mathscr{M}_{C_2} = \mathscr{M}_{C_{1h}} = \mathscr{M}_{C_{2h}} = \frac{1}{2}\left[\frac{1}{(1-t)^6} + \frac{1}{(1-t)^2\left(1-t^2\right)^2}\right] \tag{41}$$

can be computed. After building the common denominator of Eq. (41),

$$\mathscr{M}_{C_2} = \mathscr{M}_{C_{1h}} = \mathscr{M}_{C_{2h}} = \frac{1+t^2}{(1-t)^4\left(1-t^2\right)^2} \,. \tag{42}$$

follows, which is already in the desired form of Eq. (35). The corresponding Taylor series is denoted by

$$\mathscr{M}_{\text{Tay},C_2} = \mathscr{M}_{\text{Tay},C_{1h}} = \mathscr{M}_{\text{Tay},C_{2h}} = 1 + 4t + 13t^2 + 32t^3 + 70t^4 + 136^5 + 246t^6 + 416t^7 + \text{HOT} \,. \tag{43}$$

Information of Eq. (42) From the denominator in Eq. (42) it is known that a polynomially complete set of invariants contains the following primary invariants: four of degree one and two of degree two. The numerator indicates that the following secondary invariants are additionally required: the number 1 and one of degree two.[11] Since only one secondary invariant, in addition to the secondary invariant 1, is required to form a polynomially complete set of invariants, this secondary invariant must be polynomially irreducible. Consequently, the corresponding set of primary and secondary invariants constitutes an irreducible integrity basis.

Information of Eq. (43) The Taylor series (43) can be analyzed as follows. First, the constant term 1 always indicates the presence of the secondary invariant 1. The term $4t$ points out that four independent invariants exist at polynomial degree one, which are the fundamental invariants I_1, I_2, I_3 and I_4 of Tab. 3. By comparing this information with that of representation (43), it becomes evident that these invariants must also be primary invariants. With these linear invariants, ten products, I_1^2, I_2^2, I_3^2, I_4^2, I_1I_2, I_1I_3, I_1I_4, I_2I_3, I_2I_4 and I_3I_4, can be formed at quadratic degree; thus, these invariants are reducible. The term $13t^2$ then indicates that 13 independent invariants exist of quadratic degree, but since ten of them are reducible, it follows that there must be three fundamental invariants of degree two, namely I_5, I_6 and I_7. This conclusion also aligns with representation (42). Which of these three invariants is considered primary or secondary can not be concluded from the Taylor series.

From the fundamental invariants $I_1, \ldots, I_7$ of degrees one and two, 32 independent polynomially reducible invariants can be formed with cubic degree. Considering the next term, $32t^3$, we conclude that no fundamental invariant exists of cubic degree, which also follows from representation (42). At degree four, 71 products or polynomially reducible invariants can be formed from the seven fundamental invariants of lower degrees. However, the term $70t^4$ indicates that only 70 independent invariants exist at this degree. From this, we conclude that one polynomial syzygy is presented between the 71 products. Indeed, when formulated with the invariants of Tab. 3, the syzygy is

$$\begin{aligned}4I_1^4 =& -4I_5^2 + 16I_7^2 + 16I_6^2 + 4I_4^2I_5 - I_4^4 + 4I_3^2I_5 - 2I_3^2I_4^2 - I_3^4 + 32I_2I_4I_7 + 32I_2I_3I_6 + 12I_2^2I_5 + 10I_2^2I_4^2 + 10I_2^2I_3^2 \\ &- 9I_2^4 + 16I_1I_2I_5 - 8I_1I_2I_4^2 - 8I_1I_2I_3^2 - 24I_1I_2^3 + 8I_1^2I_5 - 4I_1^2I_4^2 - 4I_1^2I_3^2 - 28I_1^2I_2^2 - 16I_1^3I_2\end{aligned} \,. \tag{44}$$

In the higher polynomial degrees this counting process can be continued and would postulate that only syzygies between the fundamental invariants exist, but no new fundamental invariants. However, it should be noted that, for example, four of the syzygies at degree five can be obtained by multiplying the degree-four syzygy in Eq. (44) by the fundamental invariants I_1, I_2, I_3 and I_4 of degree one, respectively. We refer to such syzygies as primitive syzygies.

Primary invariants Given the MS in the form of Eq. (42) and the syzygy in Eq. (44), it follows directly that the invariants $I_1, I_2, I_3, I_4, I_5, I_6$ are primary invariants and I_7 is a secondary invariant. Alternatively, either I_5 or I_6 could also be chosen as secondary invariant and I_7 as primary invariant, since the syzygy (44) allows either one to be the solution of the algebraic equation.

3.5 Example: Cubic crystal system

The cubic crystal system comprises the point groups $\mathcal{T}$, $\mathcal{T}_h$, $\mathcal{O}$, $\mathcal{T}_d$ and $\mathcal{O}_h$ leading only to two different anisotropies $\mathscr{A}_{10}$ and $\mathscr{A}_{11}$ or integrity bases in hyperelasticity. It will be shown for the groups $\mathcal{T}$ and $\mathcal{T}_h$ or simply $\mathscr{A}_{10}$ how to determine an irreducible integrity basis.

Structural tensor and reducible integrity basis Since the integrity bases are equivalent for the tensor $\mathbf{C} \in \mathcal{L}^2_{\text{sym}}$ and $\mathcal{T}$ as well as $\mathcal{T}_h$, it is sufficient to only consider $\mathcal{T}_h$. The corresponding structural tensor, introduced by Zheng & Spencer (1993), is denoted as

$$^4\boldsymbol{\Lambda} = \boldsymbol{a}_1\boldsymbol{a}_1\boldsymbol{a}_2\boldsymbol{a}_2 - \boldsymbol{a}_2\boldsymbol{a}_2\boldsymbol{a}_1\boldsymbol{a}_1 + \boldsymbol{a}_3\boldsymbol{a}_3\boldsymbol{a}_1\boldsymbol{a}_1 - \boldsymbol{a}_1\boldsymbol{a}_1\boldsymbol{a}_3\boldsymbol{a}_3 + \boldsymbol{a}_2\boldsymbol{a}_2\boldsymbol{a}_3\boldsymbol{a}_3 - \boldsymbol{a}_3\boldsymbol{a}_3\boldsymbol{a}_2\boldsymbol{a}_2 \in \mathcal{L}^4 \,, \tag{45}$$

[11] From Eq. (62) it follows that one secondary invariant is always a non-zero constant, which may be chosen arbitrarily. Hence, selecting the value 1 is a legitimate choice.

where $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3 \in \mathcal{L}^1$ are orthonormal. With respect to $\mathcal{T}_h$, these 1st order tensors can be interpreted as the three two-fold axes of this group (Xiao, 1996a). To be able to determine a polynomially complete set of invariants with the table of Boehler (1977), we define the tuple of structural functions by

$$\mathcal{F}_{\mathcal{T}_h} = \left({}^4\boldsymbol{\Lambda} : \mathbf{C}, {}^4\boldsymbol{\Lambda} : \mathbf{C}^2\right) \tag{46}$$

and the tuple of argument tensors by

$$\mathcal{H}_{\mathcal{T}_h} = \left(\mathbf{C}, {}^4\boldsymbol{\Lambda} : \mathbf{C}, {}^4\boldsymbol{\Lambda} : \mathbf{C}^2\right) , \tag{47}$$

which are all symmetric 2nd order tensors. We thus obtain the 22 invariants

$$\begin{aligned}
&\mathrm{tr}[\mathbf{C}],\ \mathrm{tr}[\mathbf{C}^2],\ \mathrm{tr}[\mathbf{C}^3],\ \mathrm{tr}[{}^4\boldsymbol{\Lambda} : \mathbf{C}],\ \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C})^2],\ \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C})^3],\ \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)],\ \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^2],\ \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^3],\\
&\mathrm{tr}[\mathbf{C} \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C})],\ \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C})],\ \mathrm{tr}[\mathbf{C} \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C})^2],\ \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C})^2],\ \mathrm{tr}[\mathbf{C} \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)],\ \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)],\\
&\mathrm{tr}[\mathbf{C} \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^2],\ \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^2],\ \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C}) \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)],\ \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C})^2 \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)],\\
&\mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C}) \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^2],\ \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C})^2 \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^2],\ \mathrm{tr}[\mathbf{C} \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}) \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)] .
\end{aligned} \tag{48}$$

Irreducible integrity basis By applying the procedure outlined in Sect. 3.2 for eliminating polynomially reducible invariants, we obtain an irreducible integrity basis from the polynomially complete set of invariants in Eq. (48) for group $\mathcal{T}_h$, cf. Tab. 4. As a proof of polynomial completeness and irreducibility, the polynomial relations between the invariants from Tab. 4 and those proposed by Smith (1962) are determined using again the procedure described in Sect. 3.2. To achieve this, the orientation of the structural tensor must be aligned with that of Smith's invariants, which is why $[\boldsymbol{a}_1] = (1, 0, 0)^\top$, $[\boldsymbol{a}_2] = (0, 1, 0)^\top$ and $[\boldsymbol{a}_3] = (0, 0, 1)^\top$ are set accordingly. The polynomial relationships between the two invariant sets are presented in Tab. 38 and the comparison of the polynomial degrees between both sets in Tab. 39.

Table 4: Irreducible integrity bases for $\mathcal{T}_h$ and a tensor $\mathbf{C} \in \mathcal{L}^2_{\mathrm{sym}}$ with the structural tensor ${}^4\boldsymbol{\Lambda}$ defined by Eq. (45).

$I_1 = \mathrm{tr}[\mathbf{C}]$	$I_2 = \mathrm{tr}[\mathbf{C}^2]$	$I_3 = \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C})^2]$	$I_4 = \mathrm{tr}[\mathbf{C}^3]$	$I_5 = \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C})^3]$	$I_6 = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C})]$
$I_7 = \mathrm{tr}[\mathbf{C} \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C})^2]$	$I_8 = \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C}) \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)]$	$I_9 = \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^2]$	$I_{10} = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C})^2]$		
$I_{11} = \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C})^2 \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)]$	$I_{12} = \mathrm{tr}[\mathbf{C} \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^2]$	$I_{13} = \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C}) \cdot ({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^2]$	$I_{14} = \mathrm{tr}[({}^4\boldsymbol{\Lambda} : \mathbf{C}^2)^3]$		

Molien series Both $\mathcal{T}$ and $\mathcal{T}_h$ lead to the same MS, which is why the MS only has to be computed for $\mathcal{T}$. This group is generated by $\mathbf{Q}_{\boldsymbol{z}}^{\pi}$ and $\mathbf{Q}_{\boldsymbol{k}}^{\frac{2\pi}{3}}$ and contains twelve group elements that hold 4-times a rotational angle of $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$, 3-times an angle of π and one angle of 0. Hence, with Eqs. (26) and (34), the MS

$$\mathscr{M}_{\mathcal{T}} = \mathscr{M}_{\mathcal{T}_h} = \frac{1}{12}\left[\frac{1}{(1-t)^6} + \frac{8}{\left(1-t^3\right)^2} + \frac{3}{(1-t)^2\left(1-t^2\right)^2}\right] \tag{49}$$

can be computed. To bring the MS in the desired form (35), a multiplication with $(1+t)(1+t^2)/((1+t)(1+t^2))$ is necessary resulting in

$$\mathscr{M}_{\mathcal{T}} = \mathscr{M}_{\mathcal{T}_h} = \frac{1 + 3t^3 + 2t^4 + 2t^5 + 3t^6 + t^9}{(1-t)\left(1-t^2\right)^2\left(1-t^3\right)^2\left(1-t^4\right)} . \tag{50}$$

The corresponding Taylor series is denoted by

$$\mathscr{M}_{\mathrm{Tay},\mathcal{T}} = \mathscr{M}_{\mathrm{Tay},\mathcal{T}_h} = 1 + t + 3t^2 + 8t^3 + 14t^4 + 26t^5 + 48t^6 + 76t^7 + \mathrm{HOT} . \tag{51}$$

Information of Eq. (50) From the denominator in Eq. (50) it is known that a polynomially complete set of invariants contains the following primary invariants: one of degree one, two of degree two, two of degree three and one of degree four. The numerator tells that the following secondary invariants are additionally necessary: the secondary invariant 1 as well as three secondary invariants of degree three, two of degree four, two of degree five, three of degree six and one of degree nine.

Information of Eq. (51) The Taylor series (51) can be analyzed as follows: First, the constant term 1 indicates the presence of the secondary invariant 1, and the term t points out that one independent invariant exists at polynomial degree one, which is I_1. With this linear invariant, the product I_1^2 can be formed at quadratic degree. Thus, this invariant is reducible. The term $3t^2$ then indicates that three independent invariants exist of quadratic degree, but since I_1^2 is reducible, it follows that there must be two fundamental invariants of degree two, namely I_2 and I_3. This conclusion also aligns with representation (50). From the fundamental invariants I_1, I_2 and I_3 of degrees one and two, three independent products or polynomially reducible invariants I_1^3,

$I_1 I_2$ and $I_1 I_3$ can be formed with cubic degree. Considering the next term, $8t^3$, and subtracting the three polynomially reducible invariants, we conclude that five fundamental invariants, I_4 to I_8, exist of cubic degree. This counting process can be continued up to degree six.

At degree six, 51 products or polynomially reducible invariants can be formed from the fundamental invariants of lower degrees. However, the term $48t^6$ indicates that only 48 independent invariants exist at this degree. From this, one conclude that at least three of those 51 products are not independent and three polynomial syzygies must exist in degree six. This does not necessarily agrees with representation (50), which predicts the presence of three secondary invariants. In fact, exactly four polynomial syzygies

$$I_3 I_9 = I_8^2 + 3I_6^2 \tag{52a}$$

$$I_1 I_3 I_8 = 3I_7 I_8 + 3I_5 I_6 - 3I_3 I_{10} + I_2 I_3^2 \tag{52b}$$

$$I_1 I_3 I_6 = 3I_6 I_7 - I_5 I_8 + I_3 I_{11} \tag{52c}$$

$$2I_1^2 I_3^2 = -18I_7^2 - 6I_5^2 + I_3^3 + 12I_1 I_3 I_7 \tag{52d}$$

exist at this polynomial degree, written in the invariants of Tab. 4. Therefore, four of the polynomially reducible invariants are not independent, reducing the total number of products from 51 to 47 independent polynomially reducible invariants. However, since the Taylor series at this polynomial degree postulates 48 independent invariants, there must be one additional fundamental invariant. This in turn implies that the two remaining secondary invariants in degree six, proposed by the representation (50), are polynomially reducible secondary invariants.

The same argumentation can be applied to higher polynomial degrees. However, it should be noted that, for example, four of the syzygies at degree seven are primitive, as they can be obtained by multiplying the four degree-six syzygies in Eq. (52) by the non-trivial invariant I_1 of degree one. Similarly, the secondary invariant of degree nine is also a product of secondary invariants and is thus polynomially reducible. An irreducible integrity basis must therefore be specified without these reducible secondary invariants of degree six and nine.

Remark 9. Xiao (1996a) used an additional structural tensor ${}^4\mathbf{T}_h^a \in \mathcal{L}^4$ for $\mathcal{T}_h$, which is anti-symmetric in the first two indices and symmetric in the last two indices. The corresponding tuple of structural functions is defined by $\mathcal{F}_{\mathcal{T}_h} = \left({}^4\mathbf{\Lambda} : \mathbf{C}, {}^4\mathbf{T}_h^a : \mathbf{C}\right)$. However, this does not lead to an integrity basis when used in conjunction with the table provided by Boehler (1977), as it results in only one invariant of polynomial degree five, whereas the MS tells that two invariants of degree five are required for a polynomially complete set. This is because Boehler's basis does not necessarily constitute an integrity basis, see Remark 2. For many groups, the structural functions provided by Xiao (1996a) do lead to an integrity basis with the invariants defined by Boehler (1977), but this is not the case for $\mathcal{T}_h$, $\mathcal{T}_d$ and C_{3i} in hyperelasticity. For this reason, we choose a different tuple of structural functions in these cases.

Primary invariants Primarily, the MS indicates the polynomial degrees of the primary invariants. Furthermore, since Smith (1962) introduced a possible classification of primary and secondary invariants, a possible set of primary invariants, formulated in the fundamental invariants of Tab. 4, can be proposed by utilizing the found syzygies in Tab. 38. Thus, a set of primary invariants is given by $\left\{I_1, I_2, I_3, I_7, I_4 - I_8, I_9 + 2I_{10} - \frac{8}{3}I_1 I_4\right\}$, since the primary invariants of Smith (1962) can uniquely determined from those in this set.

Remark 10. In the absence of a known classification in primary and secondary invariants, one would need to determine the syzygies among the fundamental invariants to differentiate between primary and secondary invariants.

4 Irreducible integrity basis for all common anisotropy classes in finite strain hyperelasticity

In this section, the MS, structural tensors, structural functions and irreducible integrity bases are either calculated or provided for all relevant anisotropies $\mathscr{A}_1$-$\mathscr{A}_{14}$ in hyperelasticity. As an additional example, the anisotropy $\mathscr{A}_{15}$, arising from the icosahedral non-crystal system, is also considered. A detailed example for the monoclinic anisotropy $\mathscr{A}_2$ and cubic anisotropy $\mathscr{A}_{10}$ is presented in Sects. 3.4 and 3.5, respectively.

4.1 Molien series

For all finite groups, the MS can be computed analogously to the examples outlined in Sects. 3.4 and 3.5. In contrast, the calculation for the infinite groups is more complicated and requires transforming Eq. (26) into an integral, which is shown below. The results of the calculated series are summarized in Tab. 5.

Table 5: MS and the coefficients of their respective Taylor series up to order seven of a symmetrical second order tensor and all considered groups. (P, S, F) denotes the number of primary-, secondary- and fundamental invariants, where the number 1 is also counted as a secondary invariant.

Group/Anisotropy	Molien series	Coefficients of Taylor series	(P, S, F)
$\mathcal{C}_1, \mathcal{C}_i$ / $\mathscr{A}_1$	$\frac{1}{(1-t)^6}$	$\{1, 6, 21, 56, 126, 252, 462, 792\}$	$(6, 1, 6)$
$\mathcal{C}_2, \mathcal{C}_{1h}, \mathcal{C}_{2h}$ / $\mathscr{A}_2$	$\frac{1+t^2}{(1-t)^4(1-t^2)^2}$	$\{1, 4, 13, 32, 70, 136, 246, 416\}$	$(6, 2, 7)$
$\mathcal{D}_2, \mathcal{C}_{2v}, \mathcal{D}_{2h}$ / $\mathscr{A}_3$	$\frac{1+t^3}{(1-t)^3(1-t^2)^3}$	$\{1, 3, 9, 20, 42, 78, 138, 228\}$	$(6, 2, 7)$
$\mathcal{C}_4, \mathcal{C}_{2i}, \mathcal{C}_{4h}$ / $\mathscr{A}_4$	$\frac{1+t^2+4t^3+t^4+t^6}{(1-t)^2(1-t^2)^3(1-t^4)}$	$\{1, 2, 7, 16, 36, 68, 124, 208\}$	$(6, 8, 12)$
$\mathcal{D}_4, \mathcal{C}_{4v}, \mathcal{D}_{2d}, \mathcal{D}_{4h}$ / $\mathscr{A}_5$	$\frac{1+2t^3+t^6}{(1-t)^2(1-t^2)^3(1-t^4)}$	$\{1, 2, 6, 12, 25, 44, 77, 124\}$	$(6, 4, 8)$
$\mathcal{C}_3, \mathcal{C}_{3i}$ / $\mathscr{A}_6$	$\frac{1+2t^2+6t^3+2t^4+t^6}{(1-t)^2(1-t^2)^2(1-t^3)^2}$	$\{1, 2, 7, 20, 42, 84, 156, 264\}$	$(6, 12, 14)$
$\mathcal{D}_3, \mathcal{C}_{3v}, \mathcal{D}_{3d}$ / $\mathscr{A}_7$	$\frac{1+t^2+2t^3+t^4+t^6}{(1-t)^2(1-t^2)^2(1-t^3)^2}$	$\{1, 2, 6, 14, 28, 52, 93, 152\}$	$(6, 6, 9)$
$\mathcal{C}_6, \mathcal{C}_{3h}, \mathcal{C}_{6h}$ / $\mathscr{A}_8$	$\frac{1+3t^3+2t^4+2t^5+3t^6+t^9}{(1-t)^2(1-t^2)^2(1-t^3)(1-t^6)}$	$\{1, 2, 5, 12, 24, 46, 84, 140\}$	$(6, 12, 14)$
$\mathcal{D}_6, \mathcal{C}_{6v}, \mathcal{D}_{3h}, \mathcal{D}_{6h}$ / $\mathscr{A}_9$	$\frac{1+t^3+t^4+t^5+t^6+t^9}{(1-t)^2(1-t^2)^2(1-t^3)(1-t^6)}$	$\{1, 2, 5, 10, 19, 33, 57, 90\}$	$(6, 6, 9)$
$\mathcal{T}, \mathcal{T}_h$ / $\mathscr{A}_{10}$	$\frac{1+3t^3+2t^4+2t^5+3t^6+t^9}{(1-t)(1-t^2)^2(1-t^3)^2(1-t^4)}$	$\{1, 1, 3, 8, 14, 26, 48, 76\}$	$(6, 12, 14)$
$\mathcal{O}, \mathcal{T}_d, \mathcal{O}_h$ / $\mathscr{A}_{11}$	$\frac{1+t^3+t^4+t^5+t^6+t^9}{(1-t)(1-t^2)^2(1-t^3)^2(1-t^4)}$	$\{1, 1, 3, 6, 11, 18, 32, 48\}$	$(6, 6, 9)$
$\mathcal{C}_\infty, \mathcal{C}_{\infty h}$ / $\mathscr{A}_{12}$	$\frac{1+t^3}{(1-t)^2(1-t^2)^2(1-t^3)}$	$\{1, 2, 5, 10, 18, 30, 48, 72\}$	$(5, 2, 6)$
$\mathcal{D}_\infty, \mathcal{C}_{\infty v}, \mathcal{D}_{\infty h}$ / $\mathscr{A}_{13}$	$\frac{1}{(1-t)^2(1-t^2)^2(1-t^3)}$	$\{1, 2, 5, 9, 16, 25, 39, 56\}$	$(5, 1, 5)$
$\mathcal{K}, \mathcal{K}_h$ / $\mathscr{A}_{14}$	$\frac{1}{(1-t)(1-t^2)(1-t^3)}$	$\{1, 1, 2, 3, 4, 5, 7, 8\}$	$(3, 1, 3)$
$\mathcal{I}, \mathcal{I}_h$ / $\mathscr{A}_{15}$	$\frac{1+t^5+2t^6+t^7+t^{12}}{(1-t)(1-t^2)(1-t^3)^2(1-t^4)(1-t^5)}$	$\{1, 1, 2, 4, 6, 10, 17, 24\}$	$(6, 6, 10)$

4.1.1 Cylindrical systems

The groups $\mathcal{C}_\infty$ and $\mathcal{C}_{\infty h}$ lead to the same MS for the symmetric 2nd order tensor $\mathbf{C} \in \mathcal{L}^2_{\text{sym}}$. In order to minimize the calculation effort for the MS, group $\mathcal{C}_\infty$ is used, which contains all pure rotations $\mathbf{Q}_z^\varphi$ around an axis. To perform the calculation of the MS, Eq. (26) will be written in such a way that the definition of a Riemann integral is obtained. To do so, φ is substituted by $k\Delta\varphi$, where $k \in \mathbb{Z}_{>0}$ labels all n group elements of a given finite group $\mathcal{C}_n \approx \mathcal{C}_\infty$. To ensure that $\mathcal{C}_n$ equals $\mathcal{C}_\infty$, the limit is taken, i.e., n goes to infinity and $\Delta\varphi$ approaches zero. Hence, with the relationship $\Delta\varphi = \frac{2\pi}{n}$, Eq. (26) becomes

$$\mathscr{M}_{\mathcal{C}_\infty} := \lim_{\substack{n\to\infty \\ \Delta\varphi\to 0}} \frac{1}{n} \sum_{k=1}^{n} \frac{1}{f(k\Delta\varphi)} = \lim_{\substack{n\to\infty \\ \Delta\varphi\to 0}} \frac{1}{2\pi} \sum_{k=1}^{n} \frac{1}{f(k\Delta\varphi)} \Delta\varphi = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\varphi \, \frac{1}{f(\varphi)}. \tag{53}$$

Inserting the definition of $f(\varphi)$ from Eq. (34), the integral

$$\mathcal{M}_{C_\infty} = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\varphi \, \frac{1}{(1-t)^2(1-2t\cos(\varphi)+t^2)(1+2t-4t\cos^2(\varphi)+t^2)} \tag{54}$$

is obtained. This integral is solved with the computer algebra program Maxima (`https://maxima.sourceforge.io/`) and the final MS is presented in Tab. 5.

The point groups $\mathcal{D}_\infty$, $\mathcal{C}_{\infty v}$ and $\mathcal{D}_{\infty h}$ lead to the same MS for the symmetrical 2nd-order tensor $\mathbf{C} \in \mathcal{L}^2_{\mathrm{sym}}$. In order to minimize the calculation effort for the MS, group $\mathcal{D}_\infty$ is used, which contains all pure rotations $\mathbf{Q}_z^\varphi$ around an axis as well as all rotations $\mathbf{Q}_z^\varphi \mathbf{Q}_x^\pi$. Since $\mathbf{Q}_x^\pi$ is diagonal, the product $\mathbf{Q}_z^\varphi \mathbf{Q}_x^\pi$ is commutative. With that information it follows directly that for every $\mathbf{Q}_z^\varphi$ there exists exactly one product $\mathbf{Q}_z^\varphi \mathbf{Q}_x^\pi$ in $\mathcal{D}_\infty$. Furthermore, we note that the resulting rotation angle $\alpha(\varphi)$ of every possible product $\mathbf{Q}_z^\varphi \mathbf{Q}_x^\pi$ is always π. Hence, we distinguish between $\mathbf{Q}_z^\varphi$ and $\mathbf{Q}_z^\varphi \mathbf{Q}_x^\pi$ in $\mathcal{D}_\infty$ by splitting the MS into two sums and take the limit analogously to Eq. (53):

$$\mathcal{M}_{\mathcal{D}_\infty} := \lim_{\substack{n\to\infty \\ \Delta\varphi\to 0}} \frac{1}{2n} \sum_{k=1}^{n} \left(\frac{1}{f(k\Delta\varphi)} + \frac{1}{f(\alpha(k\Delta\varphi))} \right) = \frac{1}{2}\mathcal{M}_{C_\infty} + \frac{1}{4\pi} \int_0^{2\pi} \mathrm{d}\varphi \, \frac{1}{(1-t)^2\left(1-t^2\right)^2} \, . \tag{55}$$

The final result for the MS of $\mathcal{D}_\infty$ is presented in Tab. 5.

4.1.2 Spherical system

For the isotropic case, i.e., $\mathcal{SO}(3)$ and $\mathcal{O}(3)$, we first define the rotation angle φ in Eq. (34) as a function of the three Euler angles α, β and γ implicitly by

$$\cos[\varphi(\alpha,\beta,\gamma)] = \frac{1}{2}\left(\cos(\alpha+\gamma) + \cos(\beta) + \cos(\alpha+\gamma)\cos(\beta) - 1\right) \, , \tag{56}$$

thereby obtaining the expression

$$g\left(t, \varphi(\alpha,\beta,\gamma)\right) = (1-t)^2 \left(1 - 2t\cos\left[\varphi(\alpha,\beta,\gamma)\right] + t^2\right)\left(1 + 2t - 4t\cos^2\left[\varphi(\alpha,\beta,\gamma)\right] + t^2\right) \, . \tag{57}$$

Then, the MS can be calculated by the integral

$$\mathcal{M}_{O(3)} = \mathcal{M}_{SO(3)} = \frac{1}{8\pi^2} \int_0^{2\pi} \mathrm{d}\alpha \int_0^{\pi} \mathrm{d}\beta \int_0^{2\pi} \mathrm{d}\gamma \, \frac{\sin(\beta)}{g\left(t, \varphi(\alpha,\beta,\gamma)\right)} \, , \tag{58}$$

where $\sin(\beta)/8\pi^2$ denotes the Haar probability measure (Sturmfels, 2008). Since calculating the integral (58) is quiet challenging, the integrand is first expanded into a Taylor series

$$g(t, \varphi(\alpha,\beta,\gamma) = \sum_{i=1}^{\infty} \frac{1}{i!} \left.\frac{\mathrm{d}^i g}{dt^i}\right|_{t=0} \tag{59}$$

up to a finite order, which is then integrated term by term. This yields the MS

$$\mathcal{M}_{O(3),\mathrm{Tay}} = \mathcal{M}_{SO(3),\mathrm{Tay}} = 1 + 1t + 2t^2 + 3t^3 + 4t^4 + 5t^5 + 7t^6 + 8t^7 + \mathrm{HOT} \, . \tag{60}$$

The series (60) can subsequently be expressed in rational form

$$\mathcal{M}_{O(3)} = \mathcal{M}_{SO(3)} = \frac{1}{(1-t)\left(1-t^2\right)\left(1-t^3\right)} \, , \tag{61}$$

which indicates the existence of exactly three primary invariants in degrees one, two, and three. This is fully consistent with the well-known invariants in the isotropic case. Furthermore, Eq. (61) is also validated by Shariff (2023), who showed that the number of primary invariants is three less than the number of independent tensor coordinates in the isotropic case.

Remark 11. The maximum order to which the Taylor expansion in Eq. (60) must be carried out can be limited by the result of Spencer (1961), which states that the highest degree of a fundamental invariant for any number of non-constant 2nd order symmetric tensors is at most six. Therefore, forming the Taylor series beyond the 6th order is only meaningful if syzygies exist among the invariants of interest. However, in the isotropic case and only one symmetric second order tensor, only primary invariants are present and thus no syzygies.

Information to linear elasticity In contrast to the nonlinear theory, fewer anisotropies can be distinguished for linear elasticity. This is since quadratic energy densities have to be considered in that case and thus only invariants with polynomial degree two or less are relevant. Which anisotropies coincide can be inferred directly from the coefficients of the Taylor series in Tab. 5, as well as from the knowledge of which groups are subgroups of other groups. This is because if an invariant is invariant with respect to all transformations of a group $\mathcal{G}$, then it is also invariant with respect to all transformations of a subgroup $\mathcal{G}_{\mathrm{sub}} \subseteq \mathcal{G}$. If the number of fundamental invariants up to a given degree then matches for both groups, it is no longer possible to distinguish whether $\mathcal{G}_{\mathrm{sub}} \subseteq \mathcal{G}$ or $\mathcal{G}$ is considered from those invariants.

Consider the groups $\mathcal{T}$ and $\mathcal{O}$ as an example or equivalently speaking the two cubic anisotropies $\mathscr{A}_{10}$ and $\mathscr{A}_{11}$. We know that $\mathcal{T} \subseteq \mathcal{O}$. Thus, every $\mathcal{O}$-invariant is also a $\mathcal{T}$-invariant. Furthermore, the first three coefficients of the respective Taylor series in Tab. 5 read 1, 1 and 3 in both cases. From this it is obvious that the number of fundamental invariants are also equal up to polynomial degree two. But since the number of fundamental invariants are equal and every $\mathcal{O}$-invariant is also a $\mathcal{T}$-invariant, the fundamental invariants have to be identical up to polynomial degree two or can be chosen identical. Hence, the two cubic anisotropies $\mathscr{A}_{10}$ and $\mathscr{A}_{11}$ can not be distinguished when only considering invariants up to degree two. It should be noted that we deliberately did not choose group $\mathcal{T}_h$ and group $\mathcal{O}$ as examples, since $\mathcal{T}_h$ is not a subgroup of $\mathcal{O}$. However, as also noted in Remark 1, the invariants for a 2nd order tensor and groups $\mathcal{T}$ and $\mathcal{T}_h$ are identical. Therefore, the discussion would fall back to groups $\mathcal{T}$ and $\mathcal{O}$ anyway.

By doing this analogously for all anisotropies examined, it first follows that the four anisotropies $\mathscr{A}_8$, $\mathscr{A}_9$, $\mathscr{A}_{12}$ and $\mathscr{A}_{13}$ are indistinguishable in linear elasticity. Analogously $\mathscr{A}_{10}$ and $\mathscr{A}_{11}$ as well as $\mathscr{A}_{14}$ and $\mathscr{A}_{15}$ can not be distinguished when only fundamental invariants up to polynomial degree 2 are considered, respectively. Hence, the 15 considered anisotropies in this work reduce to 10 anisotropies in linear elasticity (Apel, 2004, Otto et al., 2025). However, regarding the elasticity tensor, $\mathscr{A}_4$ can not be distinguished from $\mathscr{A}_5$ and $\mathscr{A}_6$ not from $\mathscr{A}_7$, respectively. This is because, by rotating the elasticity tensor appropriately, the characteristic symmetries of the tensor can no longer be distinguished in these cases. Thus, only 8 anisotropies are identifiable in linear elasticity by looking at the elasticity tensor (Moakher & Norris, 2006).

4.2 Structural tensors and structural functions

Some point groups result in the same anisotropies in hyperelasticity, see Remark 1. Nevertheless, in order to provide an alternative but equivalent set of invariants in the next section, all groups studied by Xiao (1996a, 1997c, 1998b) and relevant to this work are taken into account. The definitions of the required structural tensors are listed in Tab. 6, while Tab. 7 provides an overview of the structural tensors and structural functions used for all considered groups. Furthermore, in Tabs. 8 and 9 the conversions of single structural tensors (Zheng & Spencer, 1993) to the multiple structural tensors (Xiao, 1996a) are presented. We emphasize that, for the trigonal and hexagonal crystal systems, the formulas presented in Tab. 8 refer to a specific relative orientation between the vectors associated with the respective structural tensors.

Table 6: Definitions of structural tensors ${}^n\mathbf{P}_n$, ${}^n\mathbf{P}'_n$, ${}^4\mathbf{\Lambda}$, ${}^3\mathbf{\Sigma}$ and ${}^4\mathbf{\Theta}$ from Zheng & Spencer (1993) as well as ${}^4\mathbf{D}_{4h}$, ${}^4\mathbf{D}_{3d}$, ${}^3\mathbf{D}_{3h}$, ${}^6\mathbf{D}_{6h}$, ${}^6\mathbf{I}_h$, ${}^8\mathbf{I}_h$ and ${}^{10}\mathbf{I}_h$ from Xiao (1996a, 1997c). $\boldsymbol{a}_\sigma \cdot \boldsymbol{a}_\tau = \delta_{\sigma\tau}$, $\boldsymbol{a}_3 \cdot \boldsymbol{l}_\sigma = 0$, $\boldsymbol{l}_\sigma \cdot \boldsymbol{l}_\tau \overset{\sigma\neq\tau}{=} -1/2$ and $\boldsymbol{l}_\sigma \cdot \boldsymbol{l}_\sigma = \boldsymbol{n}_\sigma \cdot \boldsymbol{n}_\sigma = 1$, where $\boldsymbol{n}_\sigma$ denotes the six five-fold axes of $\mathcal{I}_h$.

$\mathbf{P}'_2 = \boldsymbol{a}_1\boldsymbol{a}_2 + \boldsymbol{a}_2\boldsymbol{a}_1$	$\mathbf{P}_2 = \boldsymbol{a}_1\boldsymbol{a}_1 - \boldsymbol{a}_2\boldsymbol{a}_2$	${}^3\mathbf{P}'_3 = \boldsymbol{a}_1\mathbf{P}'_2 + \boldsymbol{a}_2\mathbf{P}_2$	${}^4\mathbf{P}'_4 = \mathbf{P}_2\mathbf{P}'_2 + \mathbf{P}'_2\mathbf{P}_2$	${}^4\mathbf{P}_4 = \mathbf{P}_2\mathbf{P}_2 - \mathbf{P}'_2\mathbf{P}'_2$
${}^6\mathbf{P}_6 = \mathbf{P}_2{}^4\mathbf{P}_4 - \mathbf{P}'_2{}^4\mathbf{P}'_4$	${}^4\mathbf{D}_{4h} = \sum_{\sigma=1}^{2} \overset{4}{\otimes}\boldsymbol{a}_\sigma$	${}^4\mathbf{D}_{3d} = \sum_{\sigma=1}^{3} {}^3\mathbf{E} \cdot \overset{3}{\otimes}\boldsymbol{l}_\sigma$	${}^3\mathbf{D}_{3h} = \sum_{\sigma=1}^{3} \overset{3}{\otimes}\boldsymbol{l}_\sigma$	${}^6\mathbf{D}_{6h} = \sum_{\sigma=1}^{3} \overset{6}{\otimes}\boldsymbol{l}_\sigma$
${}^6\mathbf{I}_h = \sum_{\sigma=1}^{6} \overset{6}{\otimes}\boldsymbol{n}_\sigma$	${}^8\mathbf{I}_h = \sum_{\sigma=1}^{6} \overset{8}{\otimes}\boldsymbol{n}_\sigma$	${}^{10}\mathbf{I}_h = \sum_{\sigma=1}^{6} \overset{10}{\otimes}\boldsymbol{n}_\sigma$	${}^4\mathbf{C}_{3i} = \sum_{\sigma=1}^{3} \boldsymbol{a}_3\boldsymbol{l}_\sigma\boldsymbol{l}_\sigma\boldsymbol{l}_\sigma$	${}^4\mathbf{\Theta} = \sum_{\sigma=1}^{3} \overset{4}{\otimes}\boldsymbol{a}_\sigma$
${}^3\mathbf{\Sigma} = \boldsymbol{a}_1\boldsymbol{a}_2\boldsymbol{a}_3 + \boldsymbol{a}_3\boldsymbol{a}_1\boldsymbol{a}_2 + \boldsymbol{a}_2\boldsymbol{a}_3\boldsymbol{a}_1 + \boldsymbol{a}_3\boldsymbol{a}_2\boldsymbol{a}_1 + \boldsymbol{a}_1\boldsymbol{a}_3\boldsymbol{a}_2 + \boldsymbol{a}_2\boldsymbol{a}_1\boldsymbol{a}_3$			${}^4\mathbf{C}^{\mathrm{s}}_{3i} = \frac{1}{2}\sum_{\sigma=1}^{3} (\boldsymbol{a}_3\boldsymbol{l}_\sigma\boldsymbol{l}_\sigma\boldsymbol{l}_\sigma + \boldsymbol{l}_\sigma\boldsymbol{a}_3\boldsymbol{l}_\sigma\boldsymbol{l}_\sigma)$	
${}^4\mathbf{\Lambda} = \boldsymbol{a}_1\boldsymbol{a}_1\boldsymbol{a}_2\boldsymbol{a}_2 - \boldsymbol{a}_2\boldsymbol{a}_2\boldsymbol{a}_1\boldsymbol{a}_1 + \boldsymbol{a}_2\boldsymbol{a}_2\boldsymbol{a}_3\boldsymbol{a}_3 - \boldsymbol{a}_3\boldsymbol{a}_3\boldsymbol{a}_2\boldsymbol{a}_2 + \boldsymbol{a}_3\boldsymbol{a}_3\boldsymbol{a}_1\boldsymbol{a}_1 - \boldsymbol{a}_1\boldsymbol{a}_1\boldsymbol{a}_3\boldsymbol{a}_3$				

It should be noted that, in contrast to Xiao (1996a), certain modifications were made to the selected structural tensors and structural functions for groups $\mathcal{T}_h$, $\mathcal{T}_d$ and C_{3i} to obtain an integrity basis using the table of Boehler (1977), see also Remark 9. Regarding the icosahedral group $\mathcal{I}_h$, in contrast to Xiao (1997c, 1998b), the isotropic extension functions are formulated solely based on the 6th order structural tensor.

4.3 Irreducible integrity bases

With the procedure described in Sect. 3.2, all irreducible integrity bases in Tabs. 10 and 11 are computed using the structural functions listed in Tab. 7. To demonstrate the polynomial completeness and irreducibility of the integrity bases of all groups belonging to the seven crystal systems, the polynomial relationships to the irreducible integrity bases proposed by Smith (1962) are provided in E, along with a comparison of the number of invariants at each polynomial degree, allowing application of

Table 7: Structural tensors and isotropic extension functions of a single tensor $\mathbf{C} \in \mathcal{L}^2_{\text{sym}}$ of all common anisotropies in hyperelasticity as well as the icosahedral anisotropy, see Xiao (1996a, 1997c), Zheng & Spencer (1993). Definitions of the structural tensors are provided in Tab. 6, while Tabs. 8 and 9 illustrate how the listed multiple structural tensors can be derived from the single structural tensor.

Group/Anisotropy	Single structural tensor	Multiple structural tensors	Structural functions
$\mathcal{C}_i$ / $\mathcal{G}_2$ / $\mathscr{A}_1$	$\mathbf{P}_2' + {}^3\mathbf{E}\cdot\boldsymbol{a}_1$	${}^3\mathbf{E}\cdot\boldsymbol{a}_1, {}^3\mathbf{E}\cdot\boldsymbol{a}_2$	${}^3\mathbf{E}\cdot\boldsymbol{a}_1, {}^3\mathbf{E}\cdot\boldsymbol{a}_2$
$\mathcal{C}_{1h}$ / $\mathcal{G}_3$ / $\mathscr{A}_2$	$\boldsymbol{a}_3\boldsymbol{a}_3\boldsymbol{a}_2 + {}^3\mathbf{E}\cdot\boldsymbol{a}_3\boldsymbol{a}_2$	$\boldsymbol{a}_1, \boldsymbol{a}_2$	$\boldsymbol{a}_1, \boldsymbol{a}_2$
$\mathcal{C}_{2h}$ / $\mathcal{G}_5$ / $\mathscr{A}_2$	$\mathbf{P}_2 + {}^3\mathbf{E}\cdot\boldsymbol{a}_3$	${}^3\mathbf{E}\cdot\boldsymbol{a}_3, \mathbf{P}_2$	${}^3\mathbf{E}\cdot\boldsymbol{a}_3, \mathbf{P}_2$
$\mathcal{C}_{2v}$ / $\mathcal{G}_6$ / $\mathscr{A}_3$	$\boldsymbol{a}_3\mathbf{P}_2 + \overset{3}{\otimes}\boldsymbol{a}_3$	$\mathbf{P}_2, \boldsymbol{a}_3$	$\mathbf{P}_2, \boldsymbol{a}_3$
$\mathcal{D}_{2h}$ / $\mathcal{G}_8$ / $\mathscr{A}_3$	$\mathbf{P}_2$	-	$\mathbf{P}_2$
$\mathcal{C}_{2i}$ / $\mathcal{G}_9$ / $\mathscr{A}_4$	$\boldsymbol{a}_3\mathbf{P}_2 + {}^3\mathbf{E}\cdot\mathbf{P}_2$	${}^4\mathbf{D}_{4h}, {}^3\boldsymbol{\Sigma}, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$	${}^4\mathbf{D}_{4h}:\mathbf{C}, {}^3\boldsymbol{\Sigma}:\mathbf{C}, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$
$\mathcal{C}_{4h}$ / $\mathcal{G}_{11}$ / $\mathscr{A}_4$	${}^4\mathbf{P}_4 + {}^3\mathbf{E}\cdot\overset{3}{\otimes}\boldsymbol{a}_3$	${}^4\mathbf{D}_{4h}, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$	${}^4\mathbf{D}_{4h}:\mathbf{C}, {}^4\mathbf{D}_{4h}:\mathbf{C}^2, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$
$\mathcal{C}_{4v}$ / $\mathcal{G}_{13}$ / $\mathscr{A}_5$	$\boldsymbol{a}_3{}^4\mathbf{P}_4 + \overset{5}{\otimes}\boldsymbol{a}_3$	${}^4\mathbf{D}_{4h}, \boldsymbol{a}_3$	${}^4\mathbf{D}_{4h}:\mathbf{C}, {}^4\mathbf{D}_{4h}:\mathbf{C}^2, \boldsymbol{a}_3$
$\mathcal{D}_{2d}$ / $\mathcal{G}_{12}$ / $\mathscr{A}_5$	$\boldsymbol{a}_3\mathbf{P}_2'$	${}^4\mathbf{D}_{4h}, {}^3\boldsymbol{\Sigma}, \boldsymbol{a}_3\boldsymbol{a}_3$	${}^4\mathbf{D}_{4h}:\mathbf{C}, {}^3\boldsymbol{\Sigma}:\mathbf{C}, \boldsymbol{a}_3\boldsymbol{a}_3$
$\mathcal{D}_{4h}$ / $\mathcal{G}_{15}$ / $\mathscr{A}_5$	${}^4\mathbf{P}_4$	${}^4\mathbf{D}_{4h}, \boldsymbol{a}_3\boldsymbol{a}_3$	${}^4\mathbf{D}_{4h}:\mathbf{C}, {}^4\mathbf{D}_{4h}:\mathbf{C}^2, \boldsymbol{a}_3\boldsymbol{a}_3$
$\mathcal{C}_{3i}$ / $\mathcal{G}_{17}$ / $\mathscr{A}_6$	$\boldsymbol{a}_3{}^3\mathbf{P}_3' + {}^3\mathbf{E}\cdot\overset{3}{\otimes}\boldsymbol{a}_3$	${}^4\mathbf{C}_{3i}, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$	${}^4\mathbf{C}^{\mathrm{s}}_{3i}:\mathbf{C}, {}^4\mathbf{C}^{\mathrm{s}}_{3i}:\mathbf{C}^2, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$
$\mathcal{C}_{3v}$ / $\mathcal{G}_{18}$ / $\mathscr{A}_7$	${}^3\mathbf{P}_3' + \overset{3}{\otimes}\boldsymbol{a}_3$	${}^4\mathbf{D}_{3d}, \boldsymbol{a}_3$	${}^4\mathbf{D}_{3d}:\mathbf{C}, {}^4\mathbf{D}_{3d}:\mathbf{C}^2, \boldsymbol{a}_3$
$\mathcal{D}_{3d}$ / $\mathcal{G}_{20}$ / $\mathscr{A}_7$	$\boldsymbol{a}_3{}^3\mathbf{P}_3'$	${}^4\mathbf{D}_{3d}, \boldsymbol{a}_3\boldsymbol{a}_3$	${}^4\mathbf{D}_{3d}:\mathbf{C}, {}^4\mathbf{D}_{3d}:\mathbf{C}^2, \boldsymbol{a}_3\boldsymbol{a}_3$
$\mathcal{C}_{3h}$ / $\mathcal{G}_{21}$ / $\mathscr{A}_8$	$\boldsymbol{a}_3\boldsymbol{a}_3{}^3\mathbf{P}_3' + {}^3\mathbf{E}\cdot\boldsymbol{a}_3{}^3\mathbf{P}_3'$	${}^3\mathbf{D}_{3h}, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$	${}^3\mathbf{D}_{3h}:\mathbf{C}, {}^3\mathbf{D}_{3h}:\mathbf{C}^2, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$
$\mathcal{C}_{6h}$ / $\mathcal{G}_{23}$ / $\mathscr{A}_8$	${}^6\mathbf{P}_6 + {}^3\mathbf{E}\cdot\overset{5}{\otimes}\boldsymbol{a}_3$	${}^6\mathbf{D}_{6h}, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$	${}^6\mathbf{D}_{6h}::(\mathbf{C}\mathbf{C}), {}^6\mathbf{D}_{6h}::(\mathbf{C}^2\mathbf{C}^2), {}^3\mathbf{E}\cdot\boldsymbol{a}_3$
$\mathcal{C}_{6v}$ / $\mathcal{G}_{25}$ / $\mathscr{A}_9$	$\mathbf{a}_3{}^6\mathbf{P}_6 + \overset{7}{\otimes}\boldsymbol{a}_3$	${}^6\mathbf{D}_{6h}, \boldsymbol{a}_3$	${}^6\mathbf{D}_{6h}::(\mathbf{C}\mathbf{C}), {}^6\mathbf{D}_{6h}::(\mathbf{C}^2\mathbf{C}^2), \boldsymbol{a}_3$
$\mathcal{D}_{3h}$ / $\mathcal{G}_{24}$ / $\mathscr{A}_9$	${}^3\mathbf{P}_3'$	${}^3\mathbf{D}_{3h}, \boldsymbol{a}_3\boldsymbol{a}_3$	${}^3\mathbf{D}_{3h}:\mathbf{C}, {}^3\mathbf{D}_{3h}:\mathbf{C}^2, \boldsymbol{a}_3\boldsymbol{a}_3$
$\mathcal{D}_{6h}$ / $\mathcal{G}_{27}$ / $\mathscr{A}_9$	${}^6\mathbf{P}_6$	${}^6\mathbf{D}_{6h}, \boldsymbol{a}_3\boldsymbol{a}_3$	${}^6\mathbf{D}_{6h}::(\mathbf{C}\mathbf{C}), {}^6\mathbf{D}_{6h}::(\mathbf{C}^2\mathbf{C}^2), \boldsymbol{a}_3\boldsymbol{a}_3$
$\mathcal{T}_h$ / $\mathcal{G}_{29}$ / $\mathscr{A}_{10}$	${}^4\boldsymbol{\Lambda}$	-	${}^4\boldsymbol{\Lambda}:\mathbf{C}, {}^4\boldsymbol{\Lambda}:\mathbf{C}^2$
$\mathcal{T}_d$ / $\mathcal{G}_{30}$ / $\mathscr{A}_{11}$	${}^3\boldsymbol{\Sigma}$	-	${}^3\boldsymbol{\Sigma}:\mathbf{C}, {}^3\boldsymbol{\Sigma}:\mathbf{C}^2$
$\mathcal{O}_h$ / $\mathcal{G}_{32}$ / $\mathscr{A}_{11}$	${}^4\boldsymbol{\Theta}$	-	${}^4\boldsymbol{\Theta}:\mathbf{C}, {}^4\boldsymbol{\Theta}:\mathbf{C}^2$
$\mathcal{C}_\infty$ / $\mathcal{T}_1$ / $\mathscr{A}_{12}$	$\overset{3}{\otimes}\boldsymbol{a}_3 + {}^3\mathbf{E}\cdot\boldsymbol{a}_3\boldsymbol{a}_3$	$\boldsymbol{a}_3, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$	$\boldsymbol{a}_3, {}^3\mathbf{E}\cdot\boldsymbol{a}_3$
$\mathcal{C}_{\infty h}$ / $\mathcal{T}_3$ / $\mathscr{A}_{12}$	${}^3\mathbf{E}\cdot\boldsymbol{a}_3$	-	${}^3\mathbf{E}\cdot\boldsymbol{a}_3$
$\mathcal{C}_{\infty v}$ / $\mathcal{T}_2$ / $\mathscr{A}_{13}$	$\boldsymbol{a}_3$	-	$\boldsymbol{a}_3$
$\mathcal{D}_{\infty h}$ / $\mathcal{T}_4$ / $\mathscr{A}_{13}$	$\boldsymbol{a}_3\boldsymbol{a}_3$	-	$\boldsymbol{a}_3\boldsymbol{a}_3$
$\mathcal{K}_h$ / $\mathscr{A}_{14}$	$\mathbf{1}$	-	$\mathbf{1}$
$\mathcal{I}_h$ / $\mathscr{A}_{15}$	${}^6\mathbf{I}_h$	${}^6\mathbf{I}_h, {}^8\mathbf{I}_h, {}^{10}\mathbf{I}_h$	${}^6\mathbf{I}_h::(\mathbf{C}\mathbf{C}), {}^6\mathbf{I}_h::(\mathbf{C}\mathbf{C}^2)$

Table 8: Calculation of multiple structural tensors from single structural tensors for all groups considered in Tab. 7 except $\mathcal{C}_\infty$ and $\mathcal{I}_h$. Relations between structural tensors of the latter two are presented in Tab. 9. Definitions of all structural tensors are provided in Tab. 6.
▲ $\boldsymbol{l}_1 = \boldsymbol{a}_1, \boldsymbol{l}_2 = -\frac{1}{2}\boldsymbol{a}_1 + \frac{\sqrt{3}}{2}\boldsymbol{a}_2$ and $\boldsymbol{l}_3 = -\frac{1}{2}\boldsymbol{a}_1 - \frac{\sqrt{3}}{2}\boldsymbol{a}_2$ | ▼ $\boldsymbol{l}_1 = \boldsymbol{a}_2, \boldsymbol{l}_2 = \frac{\sqrt{3}}{2}\boldsymbol{a}_1 - \frac{1}{2}\boldsymbol{a}_2$ and $\boldsymbol{l}_3 = -\frac{\sqrt{3}}{2}\boldsymbol{a}_1 - \frac{1}{2}\boldsymbol{a}_2$.

Group/Anisotropy	Single structural tensor ${}^n\mathbf{M}$	Multiple structural tensors
$\mathcal{C}_i$ / $\mathcal{G}_2$ / $\mathscr{A}_1$	$\mathbf{M} = \mathbf{P}_2' + {}^3\mathbf{E}\cdot\boldsymbol{a}_1$	${}^3\mathbf{E}\cdot\boldsymbol{a}_1 = \frac{1}{2}\left(M_{ij} - M_{ji}\right)\boldsymbol{e}_i\boldsymbol{e}_j \quad {}^3\mathbf{E}\cdot\boldsymbol{a}_2 = \frac{1}{2}\left(M_{ki}M_{jk} - M_{ik}M_{kj}\right)\boldsymbol{e}_i\boldsymbol{e}_j$
$\mathcal{C}_{1h}$ / $\mathcal{G}_3$ / $\mathscr{A}_2$ $\mathcal{C}_{2h}$ / $\mathcal{G}_5$ / $\mathscr{A}_2$	${}^3\mathbf{M} = \boldsymbol{a}_3\boldsymbol{a}_3\boldsymbol{a}_2 + {}^3\mathbf{E}\cdot\boldsymbol{a}_3\boldsymbol{a}_2$ $\mathbf{M} = \mathbf{P}_2 + {}^3\mathbf{E}\cdot\boldsymbol{a}_3$	$\boldsymbol{a}_1 = M_{ikk}\boldsymbol{e}_i \quad \boldsymbol{a}_2 = M_{kki}\boldsymbol{e}_i$ ${}^3\mathbf{E}\cdot\boldsymbol{a}_3 = \frac{1}{2}\left(M_{ij} - M_{ji}\right)\boldsymbol{e}_i\boldsymbol{e}_j \quad \mathbf{P}_2 = \frac{1}{2}\left(M_{ij} + M_{ji}\right)\boldsymbol{e}_i\boldsymbol{e}_j$
$\mathcal{C}_{2v}$ / $\mathcal{G}_6$ / $\mathscr{A}_3$	${}^3\mathbf{M} = \boldsymbol{a}_3\mathbf{P}_2 + \overset{3}{\otimes}\boldsymbol{a}_3$	$\mathbf{P}_2 = \left(M_{kkm}M_{mij} - M_{kki}M_{mmj}\right)\boldsymbol{e}_i\boldsymbol{e}_j \quad \boldsymbol{a}_3 = M_{kki}\boldsymbol{e}_i$
$\mathcal{C}_{2i}$ / $\mathcal{G}_9$ / $\mathscr{A}_4$ $\mathcal{C}_{4h}$ / $\mathcal{G}_{11}$ / $\mathscr{A}_4$	${}^3\mathbf{M} = \boldsymbol{a}_3\mathbf{P}_2 + {}^3\mathbf{E}\cdot\mathbf{P}_2$ ${}^4\mathbf{M} = {}^4\mathbf{P}_4 + {}^3\mathbf{E}\cdot\overset{3}{\otimes}\boldsymbol{a}_3$	${}^4\mathbf{D}_{4h} = \frac{1}{200}\left[4A_{im}A_{mj}A_{kn}A_{nl} + 25\left(A_{ij} - B_{ij}\right)\left(A_{kl} - B_{kl}\right)\right]\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l$ with $A_{ij} = E_{ikl}M_{klj}$ and $B_{ij} = E_{ikl}\left(M_{jkl} + M_{kjl}\right)$ ${}^3\boldsymbol{\Sigma} = \left(A_{ijk} + A_{jik} + A_{ikj}\right)\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k$ with $A_{ijk} = M_{ijk} - \frac{1}{3}\left(M_{imn}M_{lmn} - \frac{1}{2}M_{min}M_{mln}\right)M_{ljk}$ ${}^3\mathbf{E}\cdot\boldsymbol{a}_3 = \left(M_{kli} - B_{kli}\right)B_{klj}\boldsymbol{e}_i\boldsymbol{e}_j$ with $B_{kli} = \frac{1}{3}\left(M_{kmn}M_{omn} - \frac{1}{2}M_{mkn}M_{mon}\right)\left(M_{oli} + M_{loi}\right)$ ${}^4\mathbf{D}_{4h} = \frac{1}{32}\left[4\left(M_{ijkl} + M_{jikl} + M_{ijmn}M_{nmkl}\right) + M_{imno}M_{onmj}M_{kpqr}M_{rqpl}\right]\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l$ ${}^3\mathbf{E}\cdot\boldsymbol{a}_3 = M_{ijkk}\boldsymbol{e}_i\boldsymbol{e}_j$
$\mathcal{C}_{4v}$ / $\mathcal{G}_{13}$ / $\mathscr{A}_5$ $\mathcal{D}_{2d}$ / $\mathcal{G}_{12}$ / $\mathscr{A}_5$ $\mathcal{D}_{4h}$ / $\mathcal{G}_{15}$ / $\mathscr{A}_5$	${}^5\mathbf{M} = \boldsymbol{a}_3{}^4\mathbf{P}_4 + \overset{5}{\otimes}\boldsymbol{a}_3$ ${}^3\mathbf{M} = \boldsymbol{a}_3\mathbf{P}_2'$ ${}^4\mathbf{M} = {}^4\mathbf{P}_4$	${}^4\mathbf{D}_{4h} = \frac{1}{32}\left[8P_{ijkl} + 4P_{ijmn}P_{nmkl} + P_{imno}P_{onmj}P_{kpqr}P_{rqpl}\right]\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l$ with $P_{ijkl} = M_{mmnno}M_{oijkl} - M_{mmnni}M_{ooppj}M_{qqrrk}M_{ssttl}$ $\boldsymbol{a}_3 = M_{jjkki}\boldsymbol{e}_i$ ${}^4\mathbf{D}_{4h} = \frac{1}{2}\left[M_{min}M_{mnj}M_{okp}M_{opl} + M_{min}M_{mnk}M_{ojp}M_{opl} - M_{mkj}M_{mil}\right]\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l$ ${}^3\boldsymbol{\Sigma} = \left(M_{ijk} + M_{jik} + M_{kji}\right)\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k$ $\boldsymbol{a}_3\boldsymbol{a}_3 = \frac{1}{2}M_{ikl}M_{jkl}\boldsymbol{e}_i\boldsymbol{e}_j$ ${}^4\mathbf{D}_{4h} = \frac{1}{32}\left[8M_{ijkl} + 4M_{ijmn}M_{nmkl} + M_{imno}M_{onmj}M_{kpqr}M_{rqpl}\right]\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l$ $\boldsymbol{a}_3\boldsymbol{a}_3 = E_{ilk}E_{jmn}M_{mopq}M_{qpoj}M_{krst}M_{tsrn}\boldsymbol{e}_i\boldsymbol{e}_j$
$\mathcal{C}_{3i}$ / $\mathcal{G}_{17}$ / $\mathscr{A}_6$ ▼	${}^4\mathbf{M} = \boldsymbol{a}_3{}^3\mathbf{P}_3' + {}^3\mathbf{E}\cdot\overset{3}{\otimes}\boldsymbol{a}_3$	${}^4\mathbf{C}_{3i} = -\frac{3}{16}\left(4M_{ijkl} - M_{ijmm}E_{kno}M_{nopp}E_{lqr}M_{qrss}\right)\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l \quad {}^3\mathbf{E}\cdot\boldsymbol{a}_3 = M_{ijkk}\boldsymbol{e}_i\boldsymbol{e}_j$
$\mathcal{C}_{3v}$ / $\mathcal{G}_{18}$ / $\mathscr{A}_7$ ▲ $\mathcal{D}_{3d}$ / $\mathcal{G}_{20}$ / $\mathscr{A}_7$ ▲	${}^3\mathbf{M} = {}^3\mathbf{P}_3' + \overset{3}{\otimes}\boldsymbol{a}_3$ ${}^4\mathbf{M} = \boldsymbol{a}_3{}^3\mathbf{P}_3'$	${}^4\mathbf{D}_{3d} = \frac{3}{4}\left[M_{jll}M_{ikm} - M_{ill}M_{jkm} + \left(M_{ill}M_{jnn} - M_{jll}M_{inn}\right)M_{koo}M_{mpp}\right]\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_m$ $\boldsymbol{a}_3 = M_{ikk}\boldsymbol{e}_i$ ${}^4\mathbf{D}_{3d} = \frac{3}{4}\left(M_{jikl} - M_{ijkl}\right)\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l \quad \boldsymbol{a}_3\boldsymbol{a}_3 = \frac{1}{4}M_{iklm}M_{jklm}\boldsymbol{e}_i\boldsymbol{e}_j$
$\mathcal{C}_{3h}$ / $\mathcal{G}_{21}$ / $\mathscr{A}_8$ ▼ $\mathcal{C}_{6h}$ / $\mathcal{G}_{23}$ / $\mathscr{A}_8$ ▼	${}^5\mathbf{M} = \boldsymbol{a}_3\boldsymbol{a}_3{}^3\mathbf{P}_3' + {}^3\mathbf{E}\cdot\boldsymbol{a}_3{}^3\mathbf{P}_3'$ ${}^6\mathbf{M} = {}^6\mathbf{P}_6 + {}^3\mathbf{E}\cdot\overset{5}{\otimes}\boldsymbol{a}_3$	${}^3\mathbf{D}_{3h} = -\frac{3}{4}M_{mmijk}\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k \quad {}^3\mathbf{E}\cdot\boldsymbol{a}_3 = \frac{1}{8}\left(M_{ijklm}M_{nnklm} - M_{jiklm}M_{nnklm}\right)\boldsymbol{e}_i\boldsymbol{e}_j$ ${}^6\mathbf{D}_{6h} = \frac{3}{64}\left(2I_{ijklmn} - M_{ijklmn} - M_{jiklmn}\right)\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l\boldsymbol{e}_m\boldsymbol{e}_n$ with $I_{ijklmn} = \frac{2}{3}\left(I_{ij}I_{klmn} + I_{ik}I_{jlmn} + I_{il}I_{kjmn} + I_{im}I_{kljn} + I_{in}I_{klmj}\right)$, $I_{klmn} = I_{kl}I_{mn} + I_{km}I_{ln} + I_{kn}I_{ml}$ and $I_{ij} = \frac{1}{17}M_{iklmno}M_{jklmno}$ ${}^3\mathbf{E}\cdot\boldsymbol{a}_3 = M_{ijkkll}\boldsymbol{e}_i\boldsymbol{e}_j$
$\mathcal{C}_{6v}$ / $\mathcal{G}_{25}$ / $\mathscr{A}_9$ ▼ $\mathcal{D}_{3h}$ / $\mathcal{G}_{24}$ / $\mathscr{A}_9$ ▼ $\mathcal{D}_{6h}$ / $\mathcal{G}_{27}$ / $\mathscr{A}_9$ ▼	${}^7\mathbf{M} = \mathbf{a}_3{}^6\mathbf{P}_6 + \overset{7}{\otimes}\boldsymbol{a}_3$ ${}^3\mathbf{M} = {}^3\mathbf{P}_3'$ ${}^6\mathbf{M} = {}^6\mathbf{P}_6$	${}^6\mathbf{D}_{6h} = \frac{3}{32}\left(I_{ijklmn} - P_{ijklmn}\right)\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l\boldsymbol{e}_m\boldsymbol{e}_n$ with $I_{ijklmn} = \frac{2}{3}\left(I_{ij}I_{klmn} + I_{ik}I_{jlmn} + I_{il}I_{kjmn} + I_{im}I_{kljn} + I_{in}I_{klmj}\right)$, $I_{klmn} = I_{kl}I_{mn} + I_{km}I_{ln} + I_{kn}I_{ml}, \quad I_{ij} = \frac{1}{16}\left(M_{piklmno}M_{pjklmno} - A_iA_j\right)$, $P_{ijklmn} = A_rM_{rijklmn} - A_iA_jA_kA_lA_mA_n$ and $A_i = M_{jjkklli}$ $\boldsymbol{a}_3 = M_{jjkklli}\boldsymbol{e}_i$ ${}^3\mathbf{D}_{3h} = -\frac{3}{4}M_{ijk}\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k \quad \boldsymbol{a}_3\boldsymbol{a}_3 = \frac{1}{4}E_{ikl}E_{jnm}M_{kmo}M_{oln}\boldsymbol{e}_i\boldsymbol{e}_j$ ${}^6\mathbf{D}_{6h} = \frac{3}{32}\left(I_{ijklmn} - M_{ijklmn}\right)\boldsymbol{e}_i\boldsymbol{e}_j\boldsymbol{e}_k\boldsymbol{e}_l\boldsymbol{e}_m\boldsymbol{e}_n$ with $I_{ijklmn} = \frac{2}{3}\left(I_{ij}I_{klmn} + I_{ik}I_{jlmn} + I_{il}I_{kjmn} + I_{im}I_{kljn} + I_{in}I_{klmj}\right)$, $I_{klmn} = I_{kl}I_{mn} + I_{km}I_{ln} + I_{kn}I_{ml}$ and $I_{ij} = \frac{1}{16}M_{iklmno}M_{jklmno}$ $\boldsymbol{a}_3\boldsymbol{a}_3 = \left(\delta_{ij} - \frac{1}{16}M_{iklmno}M_{jklmno}\right)\boldsymbol{e}_i\boldsymbol{e}_j$

Table 9: Calculation of multiple structural tensors from single structural tensors for the groups $\mathcal{C}_\infty$ and $\mathcal{I}_h$ considered in Tab. 7. The definitions of all structural tensors are listed in Tab. 6.

Group/Anisotropy	Single structural tensor ${}^n\mathbf{M}$	Multiple structural tensors
$\mathcal{C}_\infty$ / $\mathcal{T}_1$ / $\mathscr{A}_{12}$	${}^3\mathbf{M} = \overset{3}{\otimes}\boldsymbol{a}_3 + {}^3\mathbf{E}\cdot\boldsymbol{a}_3\boldsymbol{a}_3$	$\boldsymbol{a}_3 = M_{jji}\boldsymbol{e}_i \quad {}^3\mathbf{E}\cdot\boldsymbol{a}_3 = \frac{1}{2}M_{llk}\left(M_{ijk} - M_{jik}\right)\boldsymbol{e}_i\boldsymbol{e}_j$
$\mathcal{I}_h$ / $\mathscr{A}_{15}$	${}^6\mathbf{M} = {}^6\mathbf{I}_h$	${}^8\mathbf{I}_h = \frac{1}{4}\left[5M_{abcdef}M_{ghijef} - M_{abcdee}M_{ghijff}\right]\boldsymbol{e}_a\boldsymbol{e}_b\boldsymbol{e}_c\boldsymbol{e}_d\boldsymbol{e}_g\boldsymbol{e}_h\boldsymbol{e}_i\boldsymbol{e}_j$ ${}^{10}\mathbf{I}_h = \frac{1}{16}\left[25M_{abcdef}M_{efghij}M_{ijklmn} - 4M_{abcdee}M_{ghklmn}\right.$ $\left.-5M_{abcdef}M_{ghiief}M_{jjklmn}\right]\boldsymbol{e}_a\boldsymbol{e}_b\boldsymbol{e}_c\boldsymbol{e}_d\boldsymbol{e}_g\boldsymbol{e}_h\boldsymbol{e}_k\boldsymbol{e}_l\boldsymbol{e}_m\boldsymbol{e}_n$

Proposition 3. For the integrity bases of $\mathcal{C}_\infty$, $\mathcal{C}_{\infty h}$, $\mathcal{C}_{\infty v}$, $\mathcal{D}_{\infty h}$ and $\mathcal{K}_h$, completeness and irreducibility follows directly from the corresponding MS in Tab. 5.

Table 10: Irreducible integrity bases. $\mathbf{G}_1 = {}^3\mathbf{E}\cdot\boldsymbol{a}_3$.

Group	Irreducible integrity basis
$\mathcal{C}_i$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $\quad I_2 = \mathrm{tr}[\mathbf{C}\cdot({}^3\mathbf{E}\cdot\boldsymbol{a}_1)^2]$ $\quad I_3 = \mathrm{tr}[\mathbf{C}\cdot({}^3\mathbf{E}\cdot\boldsymbol{a}_2)^2]$ $\quad I_4 = \mathrm{tr}[\mathbf{C}\cdot{}^3\mathbf{E}\cdot\boldsymbol{a}_1\cdot{}^3\mathbf{E}\cdot\boldsymbol{a}_2]$ $I_5 = \mathrm{tr}[\mathbf{C}\cdot({}^3\mathbf{E}\cdot\boldsymbol{a}_1)^2\cdot{}^3\mathbf{E}\cdot\boldsymbol{a}_2]$ $\quad I_6 = \mathrm{tr}[\mathbf{C}\cdot{}^3\mathbf{E}\cdot\boldsymbol{a}_1\cdot({}^3\mathbf{E}\cdot\boldsymbol{a}_2)^2]$
$\mathcal{C}_{1h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $\quad I_2 = \boldsymbol{a}_1\cdot\mathbf{C}\cdot\boldsymbol{a}_1$ $\quad I_3 = \boldsymbol{a}_2\cdot\mathbf{C}\cdot\boldsymbol{a}_2$ $\quad I_4 = \boldsymbol{a}_1\cdot\mathbf{C}\cdot\boldsymbol{a}_2$ $\quad I_5 = \mathrm{tr}[\mathbf{C}^2]$ $\quad I_6 = \boldsymbol{a}_1\cdot\mathbf{C}^2\cdot\boldsymbol{a}_2$ $I_7 = \boldsymbol{a}_2\cdot\mathbf{C}^2\cdot\boldsymbol{a}_2$
$\mathcal{C}_{2h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $\quad I_2 = \mathrm{tr}[\mathbf{C}\cdot\mathbf{G}_1^2]$ $\quad I_3 = \mathrm{tr}[\mathbf{C}\cdot\mathbf{P}_2]$ $\quad I_4 = \mathrm{tr}[\mathbf{C}\cdot\mathbf{P}_2\cdot\mathbf{G}_1]$ $\quad I_5 = \mathrm{tr}[\mathbf{C}^2]$ $\quad I_6 = \mathrm{tr}[\mathbf{C}^2\cdot\mathbf{P}_2]$ $I_7 = \mathrm{tr}[\mathbf{C}^2\cdot\mathbf{P}_2\cdot\mathbf{G}_1]$
$\mathcal{C}_{2v}$, $\mathcal{D}_{2h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $\quad I_2 = \mathrm{tr}[\mathbf{C}\cdot\mathbf{P}_2]$ $\quad I_3 = \mathrm{tr}[\mathbf{C}\cdot\mathbf{P}_2^2]$ $\quad I_4 = \mathrm{tr}[\mathbf{C}^2]$ $\quad I_5 = \mathrm{tr}[\mathbf{C}^2\cdot\mathbf{P}_2]$ $\quad I_6 = \mathrm{tr}[\mathbf{C}^2\cdot\mathbf{P}_2^2]$ $I_7 = \mathrm{tr}[\mathbf{C}^3]$
$\mathcal{C}_{2i}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $\quad I_2 = \mathrm{tr}[{}^4\mathbf{D}_{4h}:\mathbf{C}]$ $\quad I_3 = \mathrm{tr}[\mathbf{C}^2]$ $\quad I_4 = ({}^3\boldsymbol{\Sigma}:\mathbf{C})\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})$ $\quad I_5 = \mathrm{tr}[\mathbf{C}^2\cdot\mathbf{G}_1^2]$ $I_6 = \mathrm{tr}[\mathbf{C}\cdot({}^4\mathbf{D}_{4h}:\mathbf{C})\cdot\mathbf{G}_1]$ $\quad I_7 = \mathrm{tr}[\mathbf{C}^3]$ $\quad I_8 = \mathrm{tr}[\mathbf{C}^2\cdot\mathbf{G}_1^2\cdot\mathbf{C}\cdot\mathbf{G}_1]$ $\quad I_9 = ({}^3\boldsymbol{\Sigma}:\mathbf{C})\cdot\mathbf{C}\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})$ $I_{10} = \mathbf{C}\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})\cdot\mathbf{G}_1\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})$ $\quad I_{11} = ({}^3\boldsymbol{\Sigma}:\mathbf{C})\cdot\mathbf{C}^2\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})$ $\quad I_{12} = \mathbf{C}^2\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})\cdot\mathbf{G}_1\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})$
$\mathcal{C}_{4h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $\quad I_2 = \mathrm{tr}[{}^4\mathbf{D}_{4h}:\mathbf{C}]$ $\quad I_3 = \mathrm{tr}[\mathbf{C}^2]$ $\quad I_4 = \mathrm{tr}[({}^4\mathbf{D}_{4h}:\mathbf{C})^2]$ $\quad I_5 = \mathrm{tr}[{}^4\mathbf{D}_{4h}:\mathbf{C}^2]$ $I_6 = \mathrm{tr}[\mathbf{C}\cdot({}^4\mathbf{D}_{4h}:\mathbf{C})\cdot\mathbf{G}_1]$ $\quad I_7 = \mathrm{tr}[\mathbf{C}^3]$ $\quad I_8 = \mathrm{tr}[\mathbf{C}^2\cdot\mathbf{G}_1^2\cdot\mathbf{C}\cdot\mathbf{G}_1]$ $\quad I_9 = \mathrm{tr}[\mathbf{C}^2\cdot({}^4\mathbf{D}_{4h}:\mathbf{C})]$ $I_{10} = \mathrm{tr}[\mathbf{C}^2\cdot({}^4\mathbf{D}_{4h}:\mathbf{C})\cdot\mathbf{G}_1]$ $\quad I_{11} = \mathrm{tr}[({}^4\mathbf{D}_{4h}:\mathbf{C}^2)^2]$ $\quad I_{12} = \mathrm{tr}[\mathbf{C}^2\cdot({}^4\mathbf{D}_{4h}:\mathbf{C}^2)\cdot\mathbf{G}_1]$
$\mathcal{C}_{4v}$, $\mathcal{D}_{4h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $\quad I_2 = \mathrm{tr}[{}^4\mathbf{D}_{4h}:\mathbf{C}]$ $\quad I_3 = \mathrm{tr}[\mathbf{C}^2]$ $\quad I_4 = \mathrm{tr}[({}^4\mathbf{D}_{4h}:\mathbf{C})^2]$ $\quad I_5 = \mathrm{tr}[{}^4\mathbf{D}_{4h}:\mathbf{C}^2]$ $\quad I_6 = \mathrm{tr}[\mathbf{C}^3]$ $I_7 = \mathrm{tr}[\mathbf{C}^2\cdot({}^4\mathbf{D}_{4h}:\mathbf{C})]$ $\quad I_8 = \mathrm{tr}[({}^4\mathbf{D}_{4h}:\mathbf{C}^2)^2]$
$\mathcal{D}_{2d}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $\quad I_2 = \mathrm{tr}[{}^4\mathbf{D}_{4h}:\mathbf{C}]$ $\quad I_3 = \mathrm{tr}[\mathbf{C}^2]$ $\quad I_4 = ({}^3\boldsymbol{\Sigma}:\mathbf{C})\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})$ $\quad I_5 = \mathrm{tr}[\mathbf{C}^2\cdot\boldsymbol{a}_3\boldsymbol{a}_3]$ $I_6 = \mathrm{tr}[\mathbf{C}^3]$ $\quad I_7 = ({}^3\boldsymbol{\Sigma}:\mathbf{C})\cdot\mathbf{C}\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})$ $\quad I_8 = ({}^3\boldsymbol{\Sigma}:\mathbf{C})\cdot\mathbf{C}^2\cdot({}^3\boldsymbol{\Sigma}:\mathbf{C})$

Icosahedral system The proof of the polynomial completeness and irreducibility of the integrity basis of $\mathcal{I}_h$ given in Table 11 requires knowledge of the syzygies between the fundamental invariants. Due to their lengthy form, these will be made available as a separate file in the final publication.

By evaluating the MS of $\mathcal{I}_h$, it first follows that the invariants listed in Tab. 11 correspond in number to those expected in the respective polynomial degrees. However, one additional secondary invariant of polynomial degree 12 still needs to be identified. When the Taylor series of the MS is expanded up to degree 12, it can be concluded that there must be exactly one, two, and four syzygies in polynomial degrees 10, 11, and 12, respectively, which are identified using the proposed algorithm described in Sect. 3.2. Consequently, the missing secondary invariant of polynomial degree 12 must be a product of already existing secondary invariants. Assuming that I_1 to I_6 are primary invariants and I_7 to I_{10} are secondary invariants, then I_8^2, I_9^2, I_8I_9 and I_7I_{10} represent possible products of secondary invariants in degree 12. These four products appear in all four identified syzygies of degree 12, respectively, along with several other products which are either linear in the chosen secondary invariants, linear in a product of secondary invariants with degree less then 12 or consist solely of primary invariants. At this stage, it is essential to determine whether the products I_8^2, I_9^2, I_8I_9 and I_7I_{10} depend on each other. To investigate this, only the found coefficients of these products in the four syzygies are of interest. When the coefficients are arranged into a matrix, it turns out to be singular

Table 11: Irreducible integrity bases. $\mathbf{G}_1 = {}^3\mathbf{E} \cdot \boldsymbol{a}_3$.

Group	Irreducible integrity basis
$\mathcal{C}_{3i}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C} \cdot \mathbf{G}_1^2]$ $I_3 = \mathrm{tr}[\mathbf{C}^2]$ $I_4 = \mathrm{tr}[({}^4\mathbf{C}^{\mathrm{s}}_{3i} : \mathbf{C})^2]$ $I_5 = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{C}^{\mathrm{s}}_{3i} : \mathbf{C})]$
	$I_6 = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{C}^{\mathrm{s}}_{3i} : \mathbf{C}) \cdot \mathbf{G}_1]$ $I_7 = \mathrm{tr}[\mathbf{C}^3]$ $I_8 = \mathrm{tr}[\mathbf{C}^2 \cdot \mathbf{G}_1^2 \cdot \mathbf{C} \cdot \mathbf{G}_1]$ $I_9 = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\mathbf{C}^{\mathrm{s}}_{3i} : \mathbf{C})]$
	$I_{10} = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{C}^{\mathrm{s}}_{3i} : \mathbf{C})^2]$ $I_{11} = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{C}^{\mathrm{s}}_{3i} : \mathbf{C}^2)]$ $I_{12} = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\mathbf{C}^{\mathrm{s}}_{3i} : \mathbf{C}) \cdot \mathbf{G}_1]$
	$I_{13} = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{C}^{\mathrm{s}}_{3i} : \mathbf{C})^2 \cdot \mathbf{G}_1]$ $I_{14} = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{C}^{\mathrm{s}}_{3i} : \mathbf{C}^2) \cdot \mathbf{G}_1]$
$\mathcal{C}_{3v}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \boldsymbol{a}_3 \cdot \mathbf{C} \cdot \boldsymbol{a}_3$ $I_3 = \mathrm{tr}[\mathbf{C}^2]$ $I_4 = \mathrm{tr}[({}^4\mathbf{D}_{3d} : \mathbf{C})^2]$ $I_5 = \mathbf{C} \cdot \boldsymbol{a}_3 \cdot ({}^4\mathbf{D}_{3d} : \mathbf{C}) \cdot \boldsymbol{a}_3$ $I_6 = \mathrm{tr}[\mathbf{C}^3]$
	$I_7 = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{D}_{3d} : \mathbf{C})^2]$ $I_8 = \mathbf{C}^2 \cdot \boldsymbol{a}_3 \cdot ({}^4\mathbf{D}_{3d} : \mathbf{C}) \cdot \boldsymbol{a}_3$ $I_9 = \mathbf{C} \cdot \boldsymbol{a}_3 \cdot ({}^4\mathbf{D}_{3d} : \mathbf{C}^2) \cdot \boldsymbol{a}_3$
$\mathcal{D}_{3d}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C} \cdot \boldsymbol{a}_3\boldsymbol{a}_3]$ $I_3 = \mathrm{tr}[\mathbf{C}^2]$ $I_4 = \mathrm{tr}[({}^4\mathbf{D}_{3d} : \mathbf{C})^2]$ $I_5 = \mathrm{tr}[\mathbf{C} \cdot \boldsymbol{a}_3\boldsymbol{a}_3 \cdot ({}^4\mathbf{D}_{3d} : \mathbf{C})]$ $I_6 = \mathrm{tr}[\mathbf{C}^3]$
	$I_7 = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{D}_{3d} : \mathbf{C})^2]$ $I_8 = \mathrm{tr}[\mathbf{C}^2 \cdot \boldsymbol{a}_3\boldsymbol{a}_3 \cdot ({}^4\mathbf{D}_{3d} : \mathbf{C})]$ $I_9 = \mathrm{tr}[\mathbf{C} \cdot \boldsymbol{a}_3\boldsymbol{a}_3 \cdot ({}^4\mathbf{D}_{3d} : \mathbf{C}^2)]$
$\mathcal{C}_{3h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C} \cdot \mathbf{G}_1^2]$ $I_3 = \mathrm{tr}[\mathbf{C}^2]$ $I_4 = ({}^3\mathbf{D}_{3h} : \mathbf{C}) \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C})$ $I_5 = \mathrm{tr}[\mathbf{C}^3]$
	$I_6 = \mathrm{tr}[\mathbf{C}^2 \cdot \mathbf{G}_1^2 \cdot \mathbf{C} \cdot \mathbf{G}_1]$ $I_7 = ({}^3\mathbf{D}_{3h} : \mathbf{C}) \cdot \mathbf{C} \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C})$ $I_8 = \mathbf{C} \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}) \cdot \mathbf{G}_1 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C})$
	$I_9 = ({}^3\mathbf{D}_{3h} : \mathbf{C}) \cdot \mathbf{C}^2 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C})$ $I_{10} = \mathbf{C}^2 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}) \cdot \mathbf{G}_1 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C})$ $I_{11} = ({}^3\mathbf{D}_{3h} : \mathbf{C}^2) \cdot \mathbf{C} \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}^2)$
	$I_{12} = \mathbf{C} \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}^2) \cdot \mathbf{G}_1 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}^2)$ $I_{13} = ({}^3\mathbf{D}_{3h} : \mathbf{C}^2) \cdot \mathbf{C}^2 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}^2)$ $I_{14} = \mathbf{C}^2 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}^2) \cdot \mathbf{G}_1 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}^2)$
$\mathcal{C}_{6h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C} \cdot \mathbf{G}_1^2]$ $I_3 = \mathrm{tr}[\mathbf{C}^2]$ $I_4 = \mathrm{tr}[{}^6\mathbf{D}_{6h} :: (\mathbf{C}\mathbf{C})]$ $I_5 = \mathrm{tr}[\mathbf{C}^3]$ $I_6 = \mathrm{tr}[\mathbf{C}^2 \cdot \mathbf{G}_1^2 \cdot \mathbf{C} \cdot \mathbf{G}_1]$
	$I_7 = \mathrm{tr}[\mathbf{C} \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}\mathbf{C}))]$ $I_8 = \mathrm{tr}[\mathbf{C} \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}\mathbf{C})) \cdot \mathbf{G}_1]$ $I_9 = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}\mathbf{C}))]$
	$I_{10} = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}\mathbf{C})) \cdot \mathbf{G}_1]$ $I_{11} = \mathrm{tr}[\mathbf{C} \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}^2\mathbf{C}^2))]$ $I_{12} = \mathrm{tr}[\mathbf{C} \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}^2\mathbf{C}^2)) \cdot \mathbf{G}_1]$
	$I_{13} = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}^2\mathbf{C}^2))]$ $I_{14} = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}^2\mathbf{C}^2)) \cdot \mathbf{G}_1]$
$\mathcal{C}_{6v}, \mathcal{D}_{6h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C} \cdot \boldsymbol{a}_3\boldsymbol{a}_3]$ $I_3 = \mathrm{tr}[\mathbf{C}^2]$ $I_4 = \mathrm{tr}[{}^6\mathbf{D}_{6h} :: (\mathbf{C}\mathbf{C})]$ $I_5 = \mathrm{tr}[\mathbf{C}^3]$ $I_6 = \mathrm{tr}[\mathbf{C} \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}\mathbf{C}))]$
	$I_7 = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}\mathbf{C}))]$ $I_8 = \mathrm{tr}[\mathbf{C} \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}^2\mathbf{C}^2))]$ $I_9 = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^6\mathbf{D}_{6h} :: (\mathbf{C}^2\mathbf{C}^2))]$
$\mathcal{D}_{3h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C} \cdot \boldsymbol{a}_3\boldsymbol{a}_3]$ $I_3 = \mathrm{tr}[\mathbf{C}^2]$ $I_4 = ({}^3\mathbf{D}_{3h} : \mathbf{C}) \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C})$ $I_5 = \mathrm{tr}[\mathbf{C}^3]$
	$I_6 = ({}^3\mathbf{D}_{3h} : \mathbf{C}) \cdot \mathbf{C} \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C})$ $I_7 = ({}^3\mathbf{D}_{3h} : \mathbf{C}) \cdot \mathbf{C}^2 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C})$ $I_8 = ({}^3\mathbf{D}_{3h} : \mathbf{C}^2) \cdot \mathbf{C} \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}^2)$
	$I_9 = ({}^3\mathbf{D}_{3h} : \mathbf{C}^2) \cdot \mathbf{C}^2 \cdot ({}^3\mathbf{D}_{3h} : \mathbf{C}^2)$
$\mathcal{T}_h$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C}^2]$ $I_3 = \mathrm{tr}[({}^4\mathbf{\Lambda} : \mathbf{C})^2]$ $I_4 = \mathrm{tr}[\mathbf{C}^3]$ $I_5 = \mathrm{tr}[({}^4\mathbf{\Lambda} : \mathbf{C})^3]$ $I_6 = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\mathbf{\Lambda} : \mathbf{C})]$
	$I_7 = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{\Lambda} : \mathbf{C})^2]$ $I_8 = \mathrm{tr}[({}^4\mathbf{\Lambda} : \mathbf{C}) \cdot ({}^4\mathbf{\Lambda} : \mathbf{C}^2)]$ $I_9 = \mathrm{tr}[({}^4\mathbf{\Lambda} : \mathbf{C}^2)^2]$ $I_{10} = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\mathbf{\Lambda} : \mathbf{C})^2]$
	$I_{11} = \mathrm{tr}[({}^4\mathbf{\Lambda} : \mathbf{C})^2 \cdot ({}^4\mathbf{\Lambda} : \mathbf{C}^2)]$ $I_{12} = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{\Lambda} : \mathbf{C}^2)^2]$ $I_{13} = \mathrm{tr}[({}^4\mathbf{\Lambda} : \mathbf{C}) \cdot ({}^4\mathbf{\Lambda} : \mathbf{C}^2)^2]$ $I_{14} = \mathrm{tr}[({}^4\mathbf{\Lambda} : \mathbf{C}^2)^3]$
$\mathcal{T}_d$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C}^2]$ $I_3 = ({}^3\mathbf{\Sigma} : \mathbf{C}) \cdot ({}^3\mathbf{\Sigma} : \mathbf{C})$ $I_4 = \mathrm{tr}[\mathbf{C}^3]$ $I_5 = ({}^3\mathbf{\Sigma} : \mathbf{C}) \cdot \mathbf{C} \cdot ({}^3\mathbf{\Sigma} : \mathbf{C})$
	$I_6 = ({}^3\mathbf{\Sigma} : \mathbf{C}) \cdot ({}^3\mathbf{\Sigma} : \mathbf{C}^2)$ $I_7 = ({}^3\mathbf{\Sigma} : \mathbf{C}^2) \cdot ({}^3\mathbf{\Sigma} : \mathbf{C}^2)$ $I_8 = ({}^3\mathbf{\Sigma} : \mathbf{C}) \cdot \mathbf{C}^2 \cdot ({}^3\mathbf{\Sigma} : \mathbf{C})$
	$I_9 = ({}^3\mathbf{\Sigma} : \mathbf{C}^2) \cdot \mathbf{C} \cdot ({}^3\mathbf{\Sigma} : \mathbf{C}^2)$
$\mathcal{O}_h$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C}^2]$ $I_3 = \mathrm{tr}[({}^4\mathbf{\Theta} : \mathbf{C})^2]$ $I_4 = \mathrm{tr}[\mathbf{C}^3]$ $I_5 = \mathrm{tr}[({}^4\mathbf{\Theta} : \mathbf{C})^3]$ $I_6 = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\mathbf{\Theta} : \mathbf{C})]$
	$I_7 = \mathrm{tr}[({}^4\mathbf{\Theta} : \mathbf{C}^2)^2]$ $I_8 = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^4\mathbf{\Theta} : \mathbf{C})^2]$ $I_9 = \mathrm{tr}[\mathbf{C} \cdot ({}^4\mathbf{\Theta} : \mathbf{C}^2)^2]$
$\mathcal{C}_\infty, \mathcal{C}_{\infty h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C} \cdot \mathbf{G}_1^2]$ $I_3 = \mathrm{tr}[\mathbf{C}^2]$ $I_4 = \mathrm{tr}[\mathbf{C}^2 \cdot \mathbf{G}_1^2]$ $I_5 = \mathrm{tr}[\mathbf{C}^3]$ $I_6 = \mathrm{tr}[\mathbf{C}^2 \cdot \mathbf{G}_1^2 \cdot \mathbf{C} \cdot \mathbf{G}_1]$
$\mathcal{C}_{\infty v}$, $\mathcal{D}_{\infty h}$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C} \cdot \boldsymbol{a}_3\boldsymbol{a}_3]$ $I_3 = \mathrm{tr}[\mathbf{C}^2]$ $I_4 = \mathrm{tr}[\mathbf{C}^2 \cdot \boldsymbol{a}_3\boldsymbol{a}_3]$ $I_5 = \mathrm{tr}[\mathbf{C}^3]$
$\mathcal{K}_h$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C}^2]$ $I_3 = \mathrm{tr}[\mathbf{C}^3]$
$\mathcal{I}_h$	$I_1 = \mathrm{tr}[\mathbf{C}]$ $I_2 = \mathrm{tr}[\mathbf{C}^2]$ $I_3 = \mathrm{tr}[\mathbf{C}^3]$ $I_4 = \mathrm{tr}[\mathbf{C} \cdot ({}^6\mathbf{I}_h :: \mathbf{C}\mathbf{C})]$ $I_5 = \mathrm{tr}[({}^6\mathbf{I}_h :: \mathbf{C}\mathbf{C})^2]$
	$I_6 = \mathrm{tr}[\mathbf{C} \cdot ({}^6\mathbf{I}_h :: \mathbf{C}\mathbf{C})^2]$ $I_7 = \mathrm{tr}[\mathbf{C}^2 \cdot ({}^6\mathbf{I}_h :: \mathbf{C}\mathbf{C}^2)]$ $I_8 = \mathrm{tr}[({}^6\mathbf{I}_h :: \mathbf{C}\mathbf{C})^3]$ $I_9 = \mathrm{tr}[({}^6\mathbf{I}_h :: \mathbf{C}\mathbf{C}^2)^2]$
	$I_{10} = \mathrm{tr}[\mathbf{C} \cdot ({}^6\mathbf{I}_h :: \mathbf{C}\mathbf{C}^2)^2]$

with exactly one eigenvalue of zero, thus revealing a dependency between the four products. By using this coefficient matrix, it follows that I_9^2 depends on $I_7 I_{10}$, indicating that the missing secondary invariant is $I_7 I_{10}$. Therefore, all invariants predicted by the MS have been identified. Finally, $\{I_1, I_2, I_3, I_4, I_5, I_6\}$ denotes the set of primary invariants and $\{I_7, I_8, I_9, I_{10}, I_7 I_{10}\}$ the set of secondary invariants.

Primary invariants From the calculated MS in Tab. 5, the polynomial degrees of the primary invariants are known. By using only the information from the MS, a set of primary invariants for $\mathcal{C}_i, \mathcal{C}_{2v}, \mathcal{D}_{2h}, \mathcal{C}_{4v}, \mathcal{D}_{4h}, \mathcal{D}_{2d}, \mathcal{C}_{\infty v}, \mathcal{D}_{\infty h}, \mathcal{K}_h$ can be determined directly from the irreducible integrity basis in Tabs. 10 and 11. For groups $\mathcal{C}_{1h}, \mathcal{C}_{2h}, \mathcal{C}_\infty$ and $\mathcal{C}_{\infty h}$, the algebraic syzygies between the fundamental invariants, shown in F, are used in addition to the MS to decide which of the fundamental invariants are primary. Furthermore, primary invariants of $\mathcal{I}_h$ were already established in the last section in order to show polynomial completeness and irreducibility of the corresponding irreducible integrity basis in Tab. 11. For the remaining groups, we utilize the syzygies in E to determine a possible set of primary invariants formulated in the invariants in Tabs. 10 and 11, analogous to the example in Sect. 3.5. The corresponding primary invariants are presented in Tab. 12.

Table 12: A possible set of primary invariants for every considered group constituted by the proposed fundamental invariants of Tabs. 10 and 11. For group $\mathcal{C}_{3h}$ we use an abbreviation denoted by $Z = \frac{1}{3}(I_{11} + I_2 I_9) I_2 - \frac{3}{16} I_2 I_5 \left[(I_1 + I_2)^2 + \frac{11}{2} I_2^2 - I_3 - \frac{8}{9} I_4\right]$.

Group	Primary invariants	Group	Primary invariants
$\mathcal{C}_i$	$\{I_1, I_2, I_3, I_4, I_5, I_6\}$	$\mathcal{C}_{3h}$	$\{I_1, I_2, I_3, I_4, I_7, I_{13} + Z\}$
$\mathcal{C}_{1h}$	$\{I_1, I_2, I_3, I_4, I_5, I_6\}$	$\mathcal{C}_{6h}$	$\{I_1, I_2, I_3, I_4, I_7, I_{13} + 3I_2(I_{11} + I_2 I_9)\}$
$\mathcal{C}_{2h}$	$\{I_1, I_2, I_3, I_4, I_5, I_6\}$	$\mathcal{C}_{6v}, \mathcal{D}_{6h}$	$\{I_1, I_2, I_3, I_4, I_6, I_9\}$
$\mathcal{C}_{2v}, \mathcal{D}_{2h}$	$\{I_1, I_2, I_3, I_4, I_5, I_6\}$	$\mathcal{D}_{3h}$	$\{I_1, I_2, I_3, I_4, I_6, I_9\}$
$\mathcal{C}_{2i}$	$\left\{I_1, I_2, I_3, I_4, I_5, I_{11} + \left(I_2 - \frac{2}{3} I_1\right) I_7 - \left(\frac{1}{2} I_1 + \frac{1}{4} I_2\right) I_9\right\}$	$\mathcal{T}_h$	$\left\{I_1, I_2, I_3, I_7, I_4 - I_8, I_9 + 2I_{10} - \frac{4}{3} I_1 I_4\right\}$
$\mathcal{C}_{4h}$	$\left\{I_1, I_2, I_3, I_4, I_5, I_{11} - I_6^2 - 2I_2 I_9\right\}$	$\mathcal{T}_d$	$\left\{I_1, I_2, I_3, I_4 + \frac{3}{4} I_5, I_5 + I_6, I_7 - I_8 - \frac{8}{3} I_1 I_4\right\}$
$\mathcal{C}_{4v}, \mathcal{D}_{4h}$	$\{I_1, I_2, I_3, I_4, I_5, I_8\}$	$\mathcal{O}_h$	$\{I_1, I_2, I_3, I_5, I_4 - 3I_6, I_7 - 2I_8\}$
$\mathcal{D}_{2d}$	$\{I_1, I_2, I_3, I_4, I_5, I_8\}$	$\mathcal{C}_\infty, \mathcal{C}_{\infty h}$	$\{I_1, I_2, I_3, I_4, I_5\}$
$\mathcal{C}_{3i}$	$\{I_1, I_2, I_3, I_4, I_{10}, I_{14} + I_2 I_6\}$	$\mathcal{C}_{\infty v}, \mathcal{D}_{\infty h}$	$\{I_1, I_2, I_3, I_4, I_5\}$
$\mathcal{C}_{3v}$	$\{I_1, I_2, I_3, I_4, I_7, I_9 + (I_2 - I_1) I_5\}$	$\mathcal{K}_h$	$\{I_1, I_2, I_3\}$
$\mathcal{D}_{3d}$	$\{I_1, I_2, I_3, I_4, I_7, I_9 + (I_2 - I_1) I_5\}$	$\mathcal{I}_h$	$\{I_1, I_2, I_3, I_4, I_5, I_6\}$

5 Conclusions

In this paper we present a framework for determining polynomially complete and irreducible sets of invariants for all common anisotropies in hyperelasticity using the concept of structural tensors. Our work covers results for the 11 types of anisotropy that arise from the classical crystal systems, as well as findings for 4 additional non-crystal anisotropies derived from the cylindrical, spherical, and icosahedral symmetry systems. The resulting invariants form irreducible integrity bases and are expressed in a coordinate-free form. This allows for straight-forward differentiation in tensor notation and extraction of the orientation of the respective anisotropy directly from the structural tensors used.

The article begins by summarizing selected fundamentals of continuum mechanics, such as various measures of deformation, strain, and stress, as well as basic concepts of constitutive modeling in hyperelasticity. Based on the principle of material symmetry, the point groups of crystal systems and the most important non-crystal systems relevant to material modeling are listed. Following this, two important concepts for modeling a scalar elastic potential using invariants are introduced: a coordinate-based description and a coordinate-free one using structural tensors. Subsequently, it is discussed how polynomially complete sets of invariants can be determined from the structural tensors using well-known information about isotropic tensor functions. Polynomial irreducibility is then achieved through the presented analytical-numerical approach for determining polynomial relations between the invariants. To demonstrate polynomial completeness and irreducibility accordingly, two approaches are presented: The first uses the information provided by the associated Molien series regarding the number of invariants and the syzygies between them at each polynomial degree. The second takes advantage of the fact that, for coordinate-based invariants, irreducible integrity bases are already known for many relevant cases. Next, the proposed approach is carried out in detail exemplarily for the cases of monoclinic and cubic anisotropy. Finally, irreducible integrity bases formulated with structural tensors are given for all common anisotropies and the icosahedral anisotropy in hyperelasticity.

The provided invariant sets are of great importance for modeling anisotropic materials via the structural tensor concept using both classical approaches as well as modern techniques based on machine learning. Thereby, this work is particularly relevant because it provides, to the best of the authors' knowledge, irreducible integrity bases using the structural tensor concept for all common anisotropies in hyperelasticity for the first time. For further studies, the computed integrity can be used for the formulation of classical material models as well as neural network-based models (Fuhg et al., 2022, Kalina et al., 2024a, Klein et al., 2022, Linden et al., 2023, Linka et al., 2021, Tac et al., 2022), and analyzed with regard to properties such as polyconvexity (Ball, 1976, Ebbing, 2010). Furthermore, the provided invariants could be compared with those expressed in coordinate-based form (Smith, 1962, Smith & Rivlin, 1958) in the context of applications. Beyond the purely mechanical case, irreducible integrity bases could also be computed for coupled field problems, such as magneto-mechanics. Lastly, based on the number of primary invariants indicated by the Molien series, one may further hypothesize that, for groups of the cylindrical non-crystal system, the number of primary invariants is one element fewer than the number of independent tensor coordinates of all constitutive variables, though this remains to be proven.

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CRediT authorship contribution statement

Brain M. Riemer: Conceptualization, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **Jörg Brummund:** Conceptualization, Formal analysis, Investigation, Methodology, Visualization, Supervision, Writing – review & editing. **Karl A. Kalina:** Conceptualization, Methodology, Investigation, Visualization, Supervision, Writing – original draft, Writing – review & editing, Funding acquisition. **Abel H. G. Milor:** Formal analysis, Writing – original draft, Writing – review & editing. **Franz Dammaß:** Formal analysis, Methodology, Writing – original draft, Writing – review & editing. **Markus Kästner:** Resources, Writing – review & editing, Funding acquisition.

Usage of AI tools

In preparing this work, the authors partially used ChatGPT, a generative AI tool, to improve the readability and language of the manuscript. After using this tool, the authors reviewed and revised the content as necessary and take full responsibility for the content of the published article.

A Glossary

Throughout this paper, we use several concepts from algebra. To ease the understanding for readers with an engineering background, we briefly recapitulate the most important definitions in the following. For further reading, we refer to textbooks on algebra, e.g., Gallian (2017), Lang (2005).

A.1 Groups and generators

Definition 3 (Group)**.** Let $\mathcal{S}$ a set and $* : \mathcal{S} \times \mathcal{S} \to \mathcal{S}$ a binary operation. The pair $(\mathcal{S}, *)$ is called a group if the following axioms are met:

(G1) $(a * b) * c = a * (b * c)\ \forall\, a, b, c \in \mathcal{S}$

(G2) $\exists\, u \in \mathcal{S} :\ u * a = a * u = a\, \forall\, a \in \mathcal{S}$

(G3) $\forall a \in \mathcal{S}\ \exists\, a^{-1} \in \mathcal{S} :\ a^{-1} * a = a * a^{-1} = u$

Remark 12. To strengthen the connection to the Schoenflies notation, calligraphic letters, such as $\mathcal{G}$, are used for all groups relevant to this work. Moreover, we generally do not explicitly distinguish between algebraic structures such as groups, rings and vector spaces and their associated sets, as this convention is also common in the literature.

Definition 4 (Generators of a group)**.** Let $(\mathcal{G}, *)$ a group. A set $\mathcal{S}_{\text{gen}} \subseteq \mathcal{G}$ is called a generating set of $\mathcal{G}$, if, for every $a \in \mathcal{G}$, for some $n \in \mathbb{Z}_{\geq 0}$, there exist $s_1, \ldots, s_n$ such that for all $i \in \{1, \ldots, n\}$, $s_i \in \mathcal{S}_{\text{gen}}$ or $(s_i)^{-1} \in \mathcal{S}_{\text{gen}}$ and $a = s_1 * \cdots * s_n$. The elements of a generating set $\mathcal{G}_{\text{gen}}$ are called group generators. If $\mathcal{S}_{\text{gen}}$ is finite, $\mathcal{G}$ is called finitely generated.

Definition 5 (Minimal generating set of a group, cf. Harper (2023))**.** Let $\mathcal{G}$ be a finite group and $\mathcal{S}_{\text{gen}}$ one possible set of generators, then $\mathcal{S}_{\text{gen}}$ is said to be a minimal generating set, if no generating set exists with fewer elements than $\mathcal{S}_{\text{gen}}$.

A.2 $\mathcal{G}$-invariant polynomials and integrity bases

Definition 6 (Ring)**.** Let $\mathcal{R}$ be a set and let $+ : \mathcal{R} \times \mathcal{R} \to \mathcal{R}$ and $* : \mathcal{R} \times \mathcal{R} \to \mathcal{R}$ binary operations. The triple $(\mathcal{R}, +, *)$ is called a ring if the following axioms are true:

(R1) $(\mathcal{R}, +)$ is a group.

(R2) $a + b = b + a\, \forall\, a, b \in \mathcal{R}$

(R3) $a * (b * c) = (a * b) * c\, \forall\, a, b, c \in \mathcal{R}$

(R4) $a * (b + c) = a * b + a * c$ and $(a + b) * c = a * c + b * c\, \forall\, a, b, c \in \mathcal{R}$

Definition 7 (Polynomial ring)**.** Let $\mathbb{R}$ be the real numbers, $n \in \mathbb{Z}_{>0}$ as well as $x_1, \ldots x_n$ (formal) variables. We define:

- a monomial M in $x_1, \ldots, x_n$ as a formal multiplication of the form:
$$x_1^{\epsilon_1} \cdots x_n^{\epsilon_n} \qquad \text{with} \quad \epsilon_1, \ldots, \epsilon_n \in \mathbb{Z}_{\geq 0}$$
The degree of the monomial M is defined as $\deg(M) := \epsilon_1 + \cdots + \epsilon_n$.
- a polynomial P in x_1, ..., x_n over $\mathbb{R}$ as a linear combination of $k \in \mathbb{Z}_{\geq 0}$ monomials $M_1, \ldots, M_k$ in $x_1, \ldots, x_n$, of the form:
$$P = \lambda_1 M_1 + \cdots + \lambda_k M_k \qquad \text{with} \quad \lambda_1, \ldots, \lambda_k \in \mathbb{R} \setminus \{0\}$$
The degree of a polynomial $P \neq 0$ is defined as $\deg(P) := \max(\{\deg(M_1), \ldots, \deg(M_k)\})$.
- a homogeneous polynomial of degree $q \in \mathbb{Z}_{\geq 0}$ as a polynomial whose monomials all have the degree q.
- the polynomial ring in $x_1, \ldots, x_n$ over $\mathbb{R}$ as the ring obtained by the set of all polynomials P in $x_1, \ldots, x_n$ over $\mathbb{R}$ combined with the standard addition and multiplication. This ring is denoted by $\mathbb{R}[x_1, \ldots, x_n]$.

Using the associative and distributive laws, it can be verified that $(\mathbb{R}[x_1, \ldots, x_n], +, \cdot)$ is indeed a ring fulfilling the axioms of Def. 6.

Definition 8 (Invariant polynomials (Sturmfels, 2008))**.** Let $\mathcal{G} \subseteq \mathcal{GL}_n(\mathbb{R})$ be a subgroup of the general linear group, $n \in \mathbb{Z}_{>0}$ and $x_1, \ldots, x_n$ formal variables. The ring of $\mathcal{G}$-invariant polynomials is defined as

$$\mathbb{R}_{\mathcal{G}}[x_1, \ldots, x_n] = \left\{ I \in \mathbb{R}[x_1, \ldots, x_n] \,\middle|\, I \circ g = I\, \forall g \in \mathcal{G} \right\},$$

We refer to the elements of $\mathbb{R}_{\mathcal{G}}[x_1, \ldots, x_n]$ as $\mathcal{G}$-invariant polynomials, $\mathcal{G}$-invariants or simply invariants.

Again using the associative and distributive laws, it can be verified that $\mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n] \subseteq \mathbb{R}[x_1,\ldots,x_n]$ is a subring, since it is closed under addition and multiplication and the zero polynomial is an element of $\mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$, cf. Sturmfels (2008, Sec. 1.3).

Definition 9 (Polynomial completeness, cf. (Sturmfels, 2008))**.** Let $m,n \in \mathbb{Z}_{>0}$ and $\mathcal{I}_{\mathcal{G}} = \{I_1,\ldots,I_m\} \subseteq \mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$ a set of $\mathcal{G}$-invariant polynomials. If, for all $\tilde{I} \in \mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$, there is a polynomial $f \in \mathbb{R}[y_1,\ldots,y_m]$ such that $\tilde{I} = f(I_1,\ldots,I_m)$, i.e., every $\mathcal{G}$-invariant polynomial can be expressed as a polynomial in $I_1,\ldots,I_m$, the set $\mathcal{I}_{\mathcal{G}}$ is termed polynomially complete. A polynomially complete set $\mathcal{I}_{\mathcal{G}}$ is also referred to as a generating set for the polynomial ring $\mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$.

Definition 10 (Polynomial irreducibility, cf. (Zheng, 1994))**.** Let $m,n \in \mathbb{Z}_{>0}$ and $\mathcal{I}_{\mathcal{G}} = \{I_1,\ldots,I_m\} \subseteq \mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$ a set of $\mathcal{G}$-invariants. If there is no $k \in \{1,\ldots,m\}$ such that it exists a polynomial $g \in \mathbb{R}[y_1,\ldots,y_{k-1},y_{k+1},\ldots,y_m]$ with $I_k = g(I_1,\ldots,I_{k-1},I_{k+1},\ldots,I_m)$, i.e., no invariant can be expressed as a polynomial in the other invariants, the set $\mathcal{I}_{\mathcal{G}}$ is termed polynomially irreducible. Its elements are then referred to as polynomial irreducible invariants.

Note that different definitions of polynomial irreducibility are considered in literature, also depending on the specific context. In particular, polynomials are commonly referred to as irreducible if a nontrivial factorization does not exist, cf. (Fröberg, 1998). Furthermore, in the context of invariants, polynomial irreducibility is frequently defined only with respect to polynomially complete invariant sets, see Apel (2004), Ebbing (2010). In this case, the two aforementioned definitions become equivalent. Also note that we generally focus on homogeneous invariant polynomials throughout this work.

Definition 11 (Fundamental invariant (Ebbing, 2010, Sturmfels, 2008))**.** Let $\mathcal{I}_{\mathcal{G}}$ be a polynomially complete and irreducible set of homogeneous $\mathcal{G}$-invariant polynomials. Its elements are termed fundamental or basic invariants.

Definition 12 (Primary invariant (Sturmfels, 2008))**.** Let $m,p \in \mathbb{Z}_{>0}$ and $\mathcal{I}_{\mathcal{G}} \subseteq \mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$ be a polynomially complete and irreducible set of homogeneous $\mathcal{G}$-invariant polynomials. Furthermore, let $\tilde{\mathcal{I}}_{\mathcal{G}} = \left\{I_1,\ldots,I_p\right\} \subseteq \mathcal{I}_{\mathcal{G}}$ the largest subset whose elements are algebraically independent. Algebraically independent means that no syzygies exist in any degree among the elements of $\tilde{\mathcal{I}}_{\mathcal{G}}$, i.e., there is no homogeneous polynomial $f \in \mathbb{R}\left[y_1,\ldots,y_p\right]$ such that $f(I_1,\ldots,I_p) = 0$. The elements of $\tilde{\mathcal{I}}_{\mathcal{G}}$ are called primary invariants.

In short, primary invariants are fundamental invariants that are not only polynomially irreducible but also algebraically independent. The ring of polynomials in the primary invariants $\mathbb{R}_{\mathcal{G}}\left[I_1,\ldots,I_p\right] \subseteq \mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$ is a subring (Sturmfels, 2008). To establish a link between these two rings, we can exploit their natural vector space structure, as proven in (Sturmfels, 2008). Consider $\mathbb{R}_{\mathcal{G}}\left[I_1,\ldots,I_p\right]$ as a subspace of $\mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$. Then, for some $q \in \mathbb{Z}_{>0}$ and homogeneous polynomials $S_1,\ldots,S_q \in \mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$, it holds

$$\mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n] = \bigoplus_{i=1}^{q} S_i\, \mathbb{R}_{\mathcal{G}}\left[I_1,\ldots,I_p\right] \ , \tag{62}$$

which is also known as Hironaka decomposition.

Definition 13 (Secondary invariant (Sturmfels, 2008))**.** Let $S_1,\ldots,S_q \in \mathbb{R}_{\mathcal{G}}[x_1,\ldots,x_n]$ be homogeneous polynomials such that Eq. (62) holds. These are referred to as secondary invariants.

Definition 14 (Integrity basis (Ebbing, 2010, Smith, 1965, Smith et al., 1963))**.** A polynomially complete set of invariants is also called an integrity basis. If the set is also polynomially irreducible, it is referred to as an irreducible integrity basis.

A.3 $\mathcal{G}$-invariant functions and functional basis

Definition 15 (Functional completeness, cf. Xiao (1997a))**.** Let $\mathcal{N}$ be a set, $\mathcal{G}$ a group, $r \in \mathbb{Z}_{>0}$, $\alpha \in \{1,\ldots,r\}$ and $I_\alpha : \mathcal{N} \to \mathbb{R}$ such that $I_\alpha \circ g = I_\alpha \ \forall\, g \in \mathcal{G}$. The set $\{I_1,\ldots,I_r\}$ is termed functionally complete if, for all $x,y \in \mathcal{N}$, it holds

$$I_\alpha(x) = I_\alpha(y),\ \alpha \in \{1,\ldots,r\} \quad \Leftrightarrow \quad \exists\, g \in \mathcal{G} : y = g * x \ . \tag{63}$$

Definition 16 (Functional irreducibility, cf. Xiao (1997a))**.** Let $\mathcal{N}$ be a set, $\mathcal{G}$ a group, $r \in \mathbb{Z}_{>0}$, $\alpha \in \{1,\ldots,r\}$ and $I_\alpha : \mathcal{N} \to \mathbb{R}$ such that $I_\alpha \circ g = I_\alpha \,\forall\, g \in \mathcal{G}$ and $\{I_1,\ldots,I_r\}$ a set of invariants. Then an invariant I_α in that set is called functionally irreducible, if there exists $x,y \in \mathcal{N}$, such that

$$I_\alpha(x) \neq I_\alpha(y) \text{ and } I_\beta(x) = I_\beta(y) \text{ for each } \beta \neq \alpha,\ 1 \leq \beta \leq r \ . \tag{64}$$

If all invariants in the set are functionally irreducible, the whole set is denoted functionally irreducible.

Note that other authors, such as Boehler et al. (1994), Desmorat et al. (2019), also introduce the concept of separating functional basis. Thereby, the set of allowed states for the tensors involved in the invariants is restricted.

Definition 17 (Functional basis, cf. (Xiao, 1997a))**.** A functionally complete set is also denoted as functional basis. Furthermore, a functionally complete and functionally irreducible set is called irreducible functional basis.

Remark 13. From the two definitions of completeness and irreducibility in Defs. 9 and 10 as well as Defs. 15 and 16, respectively, it is clear that the terms completeness and irreducibility must be understood in the given context. Since this can lead to misunderstandings, we make a strict distinction between polynomial completeness or functional completeness and polynomial irreducibility or functional irreducibility. In the definitions of integrity basis and functional basis, the specific context is clear from the respective definitions for completeness and irreducibility, which is why irreducible integrity basis and irreducible functional basis can be understood as polynomial irreducible integrity basis and functionally irreducible functional basis, respectively.

B Invariant basis of Boehler

The following Tab. 13 is taken from Boehler (1977) and allows constructing a functional basis for an arbitrary number of 1st order as well as symmetric and antisymmetric 2nd order tensors. Although originally developed for the isotropic case, this result can also be applied to various anisotropies through the structural tensor concept, as discussed in Sects. 2.4.2 and 3.1.

Table 13: Isotropic invariants for any tuple $\mathcal{H}_{O(3)} = (\boldsymbol{v}_1, .., \boldsymbol{v}_a, \mathbf{A}_1, .., \mathbf{A}_b, \mathbf{W}_1, .., \mathbf{W}_c)$ with $a, b, c \in \mathbb{Z}_{\geq 0}$, $\boldsymbol{v}_\alpha \in \mathcal{L}^1$, $\mathbf{A}_\beta \in \mathcal{L}^2_{\text{sym}}$ and $\mathbf{W}_\gamma \in \mathcal{L}^2_{\text{skw}}$ from the original article by Boehler (1977). A functional basis is obtained by constructing all invariants from all unordered combinations of one, two, three, and four variables of $\mathcal{H}_{O(3)}$.

Variables	Isotropic invariants	Variables	Isotropic invariants
$\mathbf{A}$	$\text{tr}(\mathbf{A}),\ \text{tr}(\mathbf{A}^2),\ \text{tr}(\mathbf{A}^3)$	$\mathbf{A}, \mathbf{W}, \boldsymbol{v}$	$\mathbf{A}\cdot\boldsymbol{v}\cdot\mathbf{W}\cdot\boldsymbol{v},\ \mathbf{A}^2\cdot\boldsymbol{v}\cdot\mathbf{W}\cdot\boldsymbol{v},\ \mathbf{A}\cdot\mathbf{W}\cdot\boldsymbol{v}\cdot\mathbf{W}^2\cdot\boldsymbol{v}$
$\mathbf{W}$	$\text{tr}(\mathbf{W}^2)$	$\mathbf{W}_1, \mathbf{W}_2, \boldsymbol{v}$	$\mathbf{W}_1\cdot\boldsymbol{v}\cdot\mathbf{W}_2\cdot\boldsymbol{v},\ \mathbf{W}_1^2\cdot\boldsymbol{v}\cdot\mathbf{W}_2\cdot\boldsymbol{v},\ \mathbf{W}_1\cdot\boldsymbol{v}\cdot\mathbf{W}_2^2\cdot\boldsymbol{v}$
$\boldsymbol{v}$	$\boldsymbol{v}\cdot\boldsymbol{v}$	$\mathbf{W}, \boldsymbol{v}_1, \boldsymbol{v}_2$	$\boldsymbol{v}_1\cdot\mathbf{W}\cdot\boldsymbol{v}_2,\ \boldsymbol{v}_1\cdot\mathbf{W}^2\cdot\boldsymbol{v}_2$
$\mathbf{A}_1, \mathbf{A}_2$	$\text{tr}(\mathbf{A}_1\cdot\mathbf{A}_2),\ \text{tr}(\mathbf{A}_1^2\cdot\mathbf{A}_2),\ \text{tr}(\mathbf{A}_1\cdot\mathbf{A}_2^2),$ $\text{tr}(\mathbf{A}_1^2\cdot\mathbf{A}_2^2)$	$\mathbf{A}_1, \mathbf{A}_2, \mathbf{W}$	$\text{tr}(\mathbf{A}_1\cdot\mathbf{A}_2\cdot\mathbf{W}),\ \text{tr}(\mathbf{A}_1^2\cdot\mathbf{A}_2\cdot\mathbf{W}),\ \text{tr}(\mathbf{A}_1\cdot\mathbf{A}_2^2\cdot\mathbf{W}),$ $\text{tr}(\mathbf{A}_1\cdot\mathbf{W}^2\cdot\mathbf{A}_2\cdot\mathbf{W})$
$\mathbf{A}, \mathbf{W}$	$\text{tr}(\mathbf{A}\cdot\mathbf{W}^2),\ \text{tr}(\mathbf{A}^2\cdot\mathbf{W}^2),$ $\text{tr}(\mathbf{A}^2\cdot\mathbf{W}^2\cdot\mathbf{A}\cdot\mathbf{W})$	$\mathbf{A}, \mathbf{W}_1, \mathbf{W}_2$	$\text{tr}(\mathbf{A}\cdot\mathbf{W}_1\cdot\mathbf{W}_2),\ \text{tr}(\mathbf{A}\cdot\mathbf{W}_1^2\cdot\mathbf{W}_2),$ $\text{tr}(\mathbf{A}\cdot\mathbf{W}_1\cdot\mathbf{W}_2^2)$
$\mathbf{A}, \boldsymbol{v}$	$\boldsymbol{v}\cdot\mathbf{A}\cdot\boldsymbol{v},\ \boldsymbol{v}\cdot\mathbf{A}^2\cdot\boldsymbol{v}$	$\mathbf{A}_1, \mathbf{A}_2, \boldsymbol{v}$	$\mathbf{A}_1\cdot\boldsymbol{v}\cdot\mathbf{A}_2\cdot\boldsymbol{v}$
$\mathbf{W}_1, \mathbf{W}_2$	$\text{tr}(\mathbf{W}_1\cdot\mathbf{W}_2)$	$\mathbf{A}, \boldsymbol{v}_1, \boldsymbol{v}_2$	$\boldsymbol{v}_1\cdot\mathbf{A}\cdot\boldsymbol{v}_2,\ \boldsymbol{v}_1\cdot\mathbf{A}^2\cdot\boldsymbol{v}_2$
$\mathbf{W}, \boldsymbol{v}$	$\boldsymbol{v}\cdot\mathbf{W}^2\cdot\boldsymbol{v}$	$\mathbf{A}_1, \mathbf{A}_2, \boldsymbol{v}_1, \boldsymbol{v}_2$	$\mathbf{A}_1\cdot\boldsymbol{v}_1\cdot\mathbf{A}_2\cdot\boldsymbol{v}_2 - \mathbf{A}_1\cdot\boldsymbol{v}_2\cdot\mathbf{A}_2\cdot\boldsymbol{v}_1$
$\boldsymbol{v}_1, \boldsymbol{v}_2$	$\boldsymbol{v}_1\cdot\boldsymbol{v}_2$	$\mathbf{A}, \mathbf{W}, \boldsymbol{v}_1, \boldsymbol{v}_2$	$\mathbf{A}\cdot\boldsymbol{v}_1\cdot\mathbf{W}\cdot\boldsymbol{v}_2 - \mathbf{A}\cdot\boldsymbol{v}_2\cdot\mathbf{W}\cdot\boldsymbol{v}_1$
$\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3$	$\text{tr}(\mathbf{A}_1\cdot\mathbf{A}_2\cdot\mathbf{A}_3)$	$\mathbf{W}_1, \mathbf{W}_2, \boldsymbol{v}_1, \boldsymbol{v}_2$	$\mathbf{W}_1\cdot\boldsymbol{v}_1\cdot\mathbf{W}_2\cdot\boldsymbol{v}_2 - \mathbf{W}_1\cdot\boldsymbol{v}_2\cdot\mathbf{W}_2\cdot\boldsymbol{v}_1$
$\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3$	$\text{tr}(\mathbf{W}_1\cdot\mathbf{W}_2\cdot\mathbf{W}_3)$		

C Algebraic dependency between invariants of Boehler

Using an example, we demonstrate that the invariants of Boehler (1977) are not algebraically independent, see Remark 3. For two symmetric, non-constant tensors $\mathbf{A} \in \mathcal{L}^2_{\text{sym}}$ and $\mathbf{B} \in \mathcal{L}^2_{\text{sym}}$, Boehler (1977) derives the ten invariants

$$\begin{gathered} I_1 = \text{tr}[\mathbf{A}],\ I_2 = \text{tr}[\mathbf{B}],\ I_3 = \text{tr}[\mathbf{A}^2],\ I_4 = \text{tr}[\mathbf{B}^2],\ I_5 = \text{tr}[\mathbf{A}\cdot\mathbf{B}],\ I_6 = \text{tr}[\mathbf{A}^3],\ I_7 = \text{tr}[\mathbf{B}^3], \\ I_8 = \text{tr}[\mathbf{A}^2\cdot\mathbf{B}],\ I_9 = \text{tr}[\mathbf{A}\cdot\mathbf{B}^2] \text{ and } I_{10} = \text{tr}[\mathbf{A}^2\cdot\mathbf{B}^2] \end{gathered}, \tag{65}$$

which are invariant with respect to all transformations $\mathbf{Q} \in \mathcal{O}(3)$. By calculating the MS

$$\mathscr{M}_{\text{Tay},\mathcal{O}(3)} = 1 + 2t + 6t^2 + 14t^3 + 29t^4 + 56t^5 + 106t^6 + 184t^7 + 314t^8 + 516t^9 + 822t^{10} + 1276t^{11} + 1944t^{12} + \text{HOT} \tag{66}$$

for this case, it follows that the invariants in Eq. (65) form an irreducible integrity basis and satisfy a single syzygy of degree twelve. In rational form, the MS is given by

$$\mathscr{M}_{\mathcal{O}(3)} = \frac{1 + t^4 + t^8}{(1-t)^2(1-t^2)^3(1-t^3)^4}, \tag{67}$$

which implies that the invariant I_{10} of degree four must be secondary. In zero form, the syzygy is expressed as

$$\begin{aligned}
0 = &-432I_{10}^3 + I_{10}^2\left[216I_1^2I_2^2 - 324I_1^2I_4 - 648I_1I_2I_5 + 864I_1I_9 - 324I_2^2I_3 + 864I_2I_8 + 540I_3I_4 + 108I_5^2\right] + I_{10}\left[-36I_1^4I_2^4 + 108I_1^4I_2^2I_4 - 72I_1^4I_4^2\right.\\
&+ 216I_1^3I_2^3I_5 - 288I_1^3I_2^2I_9 - 360I_1^3I_2I_4I_5 + 432I_1^3I_4I_9 + 108I_1^2I_2^4I_3 - 288I_1^2I_2^3I_8 - 324I_1^2I_2^2I_3I_4 - 324I_1^2I_2^2I_5^2 + 432I_1^2I_2I_4I_8 + 864I_1^2I_2I_5I_9\\
&+ 216I_1^2I_3I_4^2 + 108I_1^2I_4I_5^2 + 72I_1^2I_7I_8 - 648I_1^2I_9^2 - 360I_1I_2^3I_3I_5 + 432I_1I_2^2I_3I_9 + 864I_1I_2^2I_5I_8 + 648I_1I_2I_3I_4I_5 - 72I_1I_2I_6I_7 - 1080I_1I_2I_8I_9\\
&- 648I_1I_3I_4I_9 - 72I_1I_3I_5I_7 + 72I_1I_4^2I_6 - 216I_1I_4I_5I_8 - 72I_2^4I_3^2 + 432I_2^3I_3I_8 + 216I_2^2I_3^2I_4 + 108I_2^2I_3I_5^2 + 72I_2^2I_6I_9 - 648I_2^2I_8^2 + 72I_2I_3^2I_7\\
&\left.-648I_2I_3I_4I_8 - 216I_2I_3I_5I_9 - 72I_2I_4I_5I_6 - 216I_3^2I_4^2 - 108I_3I_4I_5^2 - 216I_3I_7I_8 + 216I_3I_9^2 - 216I_4I_6I_9 + 216I_4I_8^2 + 216I_5I_6I_7 - 216I_5I_8I_9\right]\\
&+ I_9^3\left[144I_1^3 - 144I_6\right] + I_9^2\left[90I_1^4I_2^2 - 126I_1^4I_4 - 288I_1^3I_2I_5 - 108I_1^2I_2^2I_3 + 432I_1^2I_2I_8 + 108I_1^2I_3I_4 - 144I_1I_2^2I_6 + 288I_1I_4I_6 + 54I_2^2I_3^2\right.\\
&\left.-216I_2I_3I_8 + 288I_2I_5I_6 - 54I_3^2I_4 + 108I_8^2\right] + I_9\left[24I_1^5I_2^4 - 72I_1^5I_2^2I_4 + 12I_1^5I_2I_7 + 36I_1^5I_4^2 - 144I_1^4I_2^3I_5 + 252I_1^4I_2I_4I_5 - 36I_1^4I_5I_7 - 72I_1^3I_2^4I_3\right.\\
&+ 216I_1^3I_2^3I_8 + 216I_1^3I_2^2I_3I_4 + 216I_1^3I_2^2I_5^2 - 72I_1^3I_2I_3I_7 - 360I_1^3I_2I_4I_8 - 72I_1^3I_3I_4^2 - 72I_1^3I_4I_5^2 - 24I_1^2I_2^4I_6 + 216I_1^2I_2^3I_3I_5 + 72I_1^2I_2^2I_4I_6\\
&- 648I_1^2I_2^2I_5I_8 - 432I_1^2I_2I_3I_4I_5 + 96I_1^2I_2I_6I_7 + 216I_1^2I_3I_5I_7 - 144I_1^2I_4^2I_6 + 216I_1^2I_4I_5I_8 + 72I_1I_2^4I_3^2 - 360I_1I_2^3I_3I_8 + 144I_1I_2^3I_5I_6\\
&- 216I_1I_2^2I_3^2I_4 + 432I_1I_2^2I_8^2 + 36I_1I_2I_3^2I_7 + 648I_1I_2I_3I_4I_8 - 144I_1I_2I_4I_5I_6 + 108I_1I_3^2I_4^2 - 72I_1I_3I_7I_8 - 216I_1I_4I_8^2 - 288I_1I_5I_6I_7 - 72I_2^3I_3^2I_5\\
&\left.+216I_2^2I_3I_5I_8 - 216I_2^2I_5^2I_6 + 108I_2I_3^2I_4I_5 - 72I_2I_3I_6I_7 - 72I_2I_4I_6I_8 - 36I_3^2I_5I_7 + 72I_3I_4^2I_6 + 72I_4I_5^2I_6 + 216I_6I_7I_8\right]\\
&+ I_8^3\left[144I_2^3 - 144I_7\right] + I_8^2\left[90I_1^2I_2^4 - 108I_1^2I_2^2I_4 - 144I_1^2I_2I_7 + 54I_1^2I_4^2 - 288I_1I_2^3I_5 + 288I_1I_5I_7 - 126I_2^4I_3 + 108I_2^2I_3I_4 + 288I_2I_3I_7 - 54I_3I_4^2\right]\\
&+ I_8\left[24I_1^4I_2^5 - 72I_1^4I_2^3I_4 - 24I_1^4I_2^2I_7 + 72I_1^4I_2I_4^2 - 144I_1^3I_2^4I_5 + 216I_1^3I_2^2I_4I_5 + 144I_1^3I_2I_5I_7 - 72I_1^3I_4^2I_5 - 72I_1^2I_2^5I_3 + 216I_1^2I_2^3I_3I_4 + 216I_1^2I_2^3I_5^2\right.\\
&+ 72I_1^2I_2^2I_3I_7 - 216I_1^2I_2I_3I_4^2 - 216I_1^2I_5^2I_7 + 12I_1I_2^5I_6 + 252I_1I_2^4I_3I_5 - 72I_1I_2^3I_4I_6 - 432I_1I_2^2I_3I_4I_5 + 96I_1I_2^2I_6I_7 - 144I_1I_2I_3I_5I_7 + 36I_1I_2I_4^2I_6\\
&+ 108I_1I_3I_4^2I_5 - 72I_1I_4I_6I_7 + 36I_2^5I_3^2 - 36I_2^4I_5I_6 - 72I_2^3I_3^2I_4 - 72I_2^3I_3I_5^2 - 144I_2^2I_3^2I_7 + 216I_2^2I_4I_5I_6 + 108I_2I_3^2I_4^2 - 288I_2I_5I_6I_7 + 72I_3^2I_4I_7\\
&\left.+72I_3I_5^2I_7 - 36I_4^2I_5I_6\right]\\
&+ I_7^2\left[-2I_1^6 + 18I_1^4I_3 - 16I_1^3I_6 - 42I_1^2I_3^2 + 72I_1I_3I_6 + 6I_3^3 - 36I_6^2\right] + I_7\left[12I_1^5I_4I_5 - 12I_1^4I_2I_3I_4 - 24I_1^4I_2I_5^2 + 16I_1^3I_2^3I_6 + 48I_1^3I_2^2I_3I_5\right.\\
&- 72I_1^3I_3I_4I_5 + 48I_1^3I_5^3 - 24I_1^2I_2^3I_3^2 - 144I_1^2I_2^2I_5I_6 + 72I_1^2I_2I_3^2I_4 - 72I_1^2I_2I_3I_5^2 + 96I_1^2I_4I_5I_6 - 96I_1I_2I_3I_4I_6 + 240I_1I_2I_5^2I_6 + 36I_1I_3^2I_4I_5\\
&\left.+24I_2^3I_3^3 - 16I_2^3I_6^2 + 96I_2^2I_3I_5I_6 - 36I_2I_3^3I_4 + 72I_2I_4I_6^2 - 72I_3I_4I_5I_6 - 48I_5^3I_6\right]\\
&+ I_6^2\left[-2I_2^6 + 18I_2^4I_4 - 42I_2^2I_4^2 + 6I_4^3\right] + I_6\left[-24I_1^3I_2^2I_4^2 + 24I_1^3I_4^3 + 48I_1^2I_2^3I_4I_5 - 12I_1I_2^4I_3I_4 - 24I_1I_2^4I_5^2 + 72I_1I_2^2I_3I_4^2 - 72I_1I_2^2I_4I_5^2 - 36I_1I_3I_4^3\right.\\
&\left.+12I_2^5I_3I_5 - 72I_2^3I_3I_4I_5 + 48I_2^3I_5^3 + 36I_2I_3I_4^2I_5\right]\\
&- 48I_5^3I_1^3I_2^3 + I_5^2\left[51I_1^4I_2^4 - 90I_1^4I_2^2I_4 + 27I_1^4I_4^2 - 90I_1^2I_2^4I_3 + 216I_1^2I_2^2I_3I_4 - 54I_1^2I_3I_4^2 + 27I_2^4I_3^2 - 54I_2^2I_3^2I_4 + 27I_3^2I_4^2\right] + I_5\left[-18I_1^5I_2^5 + 60I_1^5I_2^3I_4\right.\\
&\left.-54I_1^5I_2I_4^2 + 60I_1^3I_2^5I_3 - 216I_1^3I_2^3I_3I_4 + 180I_1^3I_2I_3I_4^2 - 54I_1I_2^5I_3^2 + 180I_1I_2^3I_3^2I_4 - 162I_1I_2I_3^2I_4^2\right]\\
&+ I_4^3\left[-3I_1^6 + 9I_1^4I_3 - 27I_1^2I_3^2 + 27I_3^3\right] + I_4^2\left[12I_1^6I_2^2 - 45I_1^4I_2^2I_3 + 54I_1^2I_2^2I_3^2 - 27I_2^2I_3^3\right] + I_4\left[-9I_1^6I_2^4 + 39I_1^4I_2^4I_3 - 45I_1^2I_2^4I_3^2 + 9I_2^4I_3^3\right]\\
&- 3I_3^3I_2^6 + 12I_3^2I_1^2I_2^6 - 9I_3I_1^4I_2^6\\
&+ 2I_1^6I_2^6
\end{aligned} \tag{68}$$

Pennisi & Trovato (1987) evaluated the invariants I_1 to I_{10} for two different states,

$$\begin{aligned}
&\text{State 1:}\quad [\mathbf{A}] = [\mathbf{A}_1] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \text{and} \quad [\mathbf{B}] = [\mathbf{B}_1] = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 0 & 0 \\ 2 & 0 & 0 \end{pmatrix} \\
&\text{State 2:}\quad [\mathbf{A}] = [\mathbf{A}_2] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \text{and} \quad [\mathbf{B}] = [\mathbf{B}_2] = \begin{pmatrix} 0 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{2} \\ \sqrt{3} & \sqrt{2} & 0 \end{pmatrix}.
\end{aligned} \tag{69}$$

The values of the invariants are identical for both states, except for I_{10}. When the invariants in Eq. (68) are evaluated for the states (69) excluding I_{10}, the cubic equation

$$0 = -432I_{10}^3 + 10800I_{10}^2 - 82512I_{10} + 196560 \tag{70}$$

results. This equation has exactly three solutions $I_{10} \in \{5, 7, 13\}$, where $I_{10}(\mathbf{A}_1, \mathbf{B}_1) = 5$ and $I_{10}(\mathbf{A}_2, \mathbf{B}_2) = 7$ are two solutions obtained by Pennisi & Trovato (1987). Consequently, the invariants of Boehler (1977) are not algebraically independent.

D Invariant sets of Smith in coordinate-based form

Several references are made to the invariants introduced by Smith (1962), who provided irreducible integrity bases for the anisotropies arising from the seven crystal systems in hyperelasticity. The invariants in coordinate-dependent form given in the Tabs. 14 to 20 below are directly taken from the original article.

Table 14: Irreducible integrity bases of a symmetric second order tensor for the triclinic system proposed by Smith (1962). The orientation of the invariants of C_1 and C_i is defined by the generator $\mathbf{1}$.

Point group	Irreducible integrity basis					
C_1, C_i	$K_1 = C_{11}$	$K_2 = C_{22}$	$K_3 = C_{33}$	$K_4 = C_{23}$	$K_5 = C_{13}$	$K_6 = C_{12}$

Table 15: Irreducible integrity bases of a symmetric second order tensor for the monoclinic system proposed by Smith (1962). The orientation of the invariants of C_2, C_{1h} and C_{2h} is defined by the generator $\mathbf{Q}_x^{\pi}$.

Point group	Irreducible integrity basis						
C_2, C_{1h}, C_{2h}	$K_1 = C_{11}$	$K_2 = C_{22}$	$K_3 = C_{33}$	$K_4 = C_{23}$	$K_5 = C_{13}^2$	$K_6 = C_{12}^2$	$L_1 = C_{12}C_{13}$

E Polynomial relations between the structural tensor-based invariants and the invariants by Smith

To demonstrate completeness and irreducibility of the integrity bases presented in Tabs. 10 and 11, we apply Propositions 1 and 3. Accordingly, the polynomial relations between the invariants in Tabs. 10 and 11 and those introduced by Smith (1962) are provided in Tabs. 21 to 38, while Tab. 39 lists the number of invariants by polynomial degree for our and Smith's invariants. For reference, Smith's invariants are also given in D.

Table 16: Irreducible integrity bases of a symmetric second order tensor for the rhombic system proposed by Smith (1962). The orientation of the invariants of $\mathcal{D}_2$, $\mathcal{C}_{2v}$ and $\mathcal{D}_{2h}$ is defined by the generators $\mathbf{Q}_x^{\pi}$ and $\mathbf{Q}_z^{\pi}$.

Point group	Irreducible integrity basis
$\mathcal{D}_2, \mathcal{C}_{2v}, \mathcal{D}_{2h}$	$K_1 = C_{11}$ $\quad K_2 = C_{22}$ $\quad K_3 = C_{33}$ $\quad K_4 = C_{23}^2$ $\quad K_5 = C_{13}^2$ $\quad K_6 = C_{12}^2$ $\quad L_1 = C_{12}C_{13}C_{23}$

Table 17: Irreducible integrity bases of a symmetric second order tensor for the tetragonal system proposed by Smith (1962). The orientation of the invariants of $\mathcal{C}_4$, $\mathcal{C}_{2i}$ and $\mathcal{C}_{4h}$ is defined by the generator $\mathbf{Q}_z^{\frac{\pi}{2}}$ and of $\mathcal{D}_4$, $\mathcal{C}_{4v}$, $\mathcal{D}_{2d}$ and $\mathcal{D}_{4h}$ by the generators $\mathbf{Q}_z^{\frac{\pi}{2}}$ and $\mathbf{Q}_x^{\pi}$.

Point group	Irreducible integrity basis
$\mathcal{C}_4, \mathcal{C}_{2i}, \mathcal{C}_{4h}, \mathcal{D}_4, \mathcal{C}_{4v}, \mathcal{D}_{2d}, \mathcal{D}_{4h}$	$K_1 = C_{11} + C_{22}$ $\quad K_2 = C_{11}C_{22}$ $\quad K_3 = C_{33}$ $\quad K_4 = C_{13}^2 + C_{23}^2$ $\quad K_5 = C_{13}^2C_{23}^2$ $\quad K_6 = C_{12}^2$ $L_1 = C_{12}C_{13}C_{23}$ $\quad L_2 = C_{11}C_{23}^2 + C_{22}C_{13}^2$
$\mathcal{C}_4, \mathcal{C}_{2i}, \mathcal{C}_{4h}$	$L_3 = C_{12}\left(C_{11} - C_{22}\right)$ $\quad L_4 = C_{12}\left(C_{13}^2 - C_{23}^2\right)$ $\quad L_5 = C_{13}C_{23}\left(C_{11} - C_{22}\right)$ $L_6 = C_{13}C_{23}\left(C_{13}^2 - C_{23}^2\right)$

Table 18: Irreducible integrity bases of a symmetric second order tensor for the trigonal systems proposed by Smith (1962). The orientation of the invariants of $\mathcal{C}_3$ and $\mathcal{C}_{3i}$ is defined by the generator $\mathbf{Q}_z^{\frac{2\pi}{3}}$ and of $\mathcal{D}_3$, $\mathcal{C}_{3v}$, $\mathcal{D}_{3d}$ by the generators $\mathbf{Q}_z^{\frac{2\pi}{3}}$ and $\mathbf{Q}_x^{\pi}$.

Point group	Irreducible integrity basis
$\mathcal{C}_3, \mathcal{C}_{3i}, \mathcal{D}_3, \mathcal{C}_{3v}, \mathcal{D}_{3d}$	$K_1 = C_{11} + C_{22}$ $\quad K_2 = C_{11}C_{22} - C_{12}^2$ $\quad K_3 = C_{11}\left(\left(C_{11} + 3C_{22}\right)^2 - 12C_{12}^2\right)$ $\quad K_4 = C_{33}$ $K_5 = C_{13}^2 + C_{23}^2$ $\quad K_6 = C_{23}\left(C_{23}^2 - 3C_{13}^2\right)$ $\quad L_1 = \left(C_{11} - C_{22}\right)C_{23} + 2C_{12}C_{13}$ $L_2 = C_{11}C_{13}^2 + C_{22}C_{23}^2 + 2C_{12}C_{13}C_{23}$ $\quad L_3 = C_{23}\left(\left(C_{11} + C_{22}\right)^2 - 4\left(C_{22}^2 - C_{12}^2\right)\right) + 8C_{11}C_{12}C_{13}$
$\mathcal{C}_3, \mathcal{C}_{3i}$	$L_4 = \left(C_{11} - C_{22}\right)C_{13} - 2C_{12}C_{23}$ $\quad L_5 = 3\left(C_{11} - C_{22}\right)^2C_{12} - 4C_{12}^3$ $\quad L_6 = C_{13}\left(C_{13}^2 - 3C_{23}^2\right)$ $L_7 = C_{13}\left(\left(C_{11} + C_{22}\right)^2 - 4\left(C_{22}^2 - C_{12}^2\right)\right) - 8C_{11}C_{12}C_{23}$ $\quad L_8 = \left(C_{11} - C_{22}\right)C_{13}C_{23} + C_{12}\left(C_{23}^2 - C_{13}^2\right)$

Table 19: Irreducible integrity bases of a symmetric second order tensor for the hexagonal systems proposed by Smith (1962). The orientation of the invariants of $\mathcal{C}_6$, $\mathcal{C}_{3h}$ and $\mathcal{C}_{6h}$ is defined by the generator $\mathbf{Q}_z^{\frac{\pi}{3}}$ and of $\mathcal{D}_6$, $\mathcal{C}_{6v}$, $\mathcal{D}_{3h}$ and $\mathcal{D}_{6h}$ by the generators $\mathbf{Q}_z^{\frac{\pi}{3}}$ and $\mathbf{Q}_x^{\pi}$.

Point group	Irreducible integrity basis
$\mathcal{C}_6, \mathcal{C}_{3h}, \mathcal{C}_{6h}, \mathcal{D}_6, \mathcal{C}_{6v}, \mathcal{D}_{3h}, \mathcal{D}_{6h}$	$K_1 = C_{11} + C_{22}$ $\quad K_2 = C_{11}C_{22} - C_{12}^2$ $\quad K_3 = C_{11}\left(\left(C_{11} + 3C_{22}\right)^2 - 12C_{12}^2\right)$ $\quad K_4 = C_{13}^2 + C_{23}^2$ $K_5 = C_{33}$ $\quad K_6 = C_{13}^2\left(C_{13}^2 - 3C_{23}^2\right)^2$ $\quad L_1 = C_{11}C_{23}^2 + C_{22}C_{13}^2 - 2C_{23}C_{13}C_{12}$ $L_2 = C_{11}\left(C_{13}^4 + 3C_{23}^4\right) + 2C_{22}C_{13}^2\left(C_{13}^2 + 3C_{23}^2\right) - 8C_{12}C_{13}^3C_{23}$ $L_3 = C_{13}^2\left(\left(C_{11} + C_{22}\right)^2 - 4\left(C_{22}^2 - C_{12}^2\right)\right) - 2C_{11}\left(\left(C_{11} + 3C_{22}\right)\left(C_{13}^2 + C_{23}^2\right) - 4C_{12}C_{13}C_{23}\right)$
$\mathcal{C}_6, \mathcal{C}_{3h}, \mathcal{C}_{6h}$	$L_4 = C_{12}\left(C_{13}^2 - C_{23}^2\right) + \left(C_{22} - C_{11}\right)C_{13}C_{23}$ $\quad L_5 = 3C_{12}\left(C_{11} - C_{22}\right)^2 - 4C_{12}^3$ $L_6 = C_{13}C_{23}\left(3\left(C_{13}^2 - C_{23}^2\right)^2 - 4C_{13}^2C_{23}^2\right)$ $L_7 = C_{13}C_{23}\left(\left(C_{11} + C_{22}\right)^2 - 4\left(C_{22}^2 - C_{12}^2\right)\right) + 4C_{11}C_{12}\left(C_{23}^2 - C_{13}^2\right)$ $L_8 = C_{12}\left(\left(C_{13}^2 + C_{23}^2\right)^2 + 4C_{23}^2\left(C_{13}^2 - C_{23}^2\right)\right) - 4C_{13}^3C_{23}\left(C_{11} - C_{22}\right)$

Table 20: Irreducible integrity bases of a symmetric second order tensor for the cubic systems proposed by Smith (1962). The orientation of the invariants of $\mathcal{T}$ and $\mathcal{T}_h$ is defined by the generators $\mathbf{Q}_{\boldsymbol{k}}^{\frac{2\pi}{3}}$ and $\mathbf{Q}_z^{\pi}$ and of $\mathcal{O}$, $\mathcal{T}_d$ and $\mathcal{O}_h$ by the generators $\mathbf{Q}_z^{\frac{\pi}{2}}$ and $\mathbf{Q}_x^{\frac{\pi}{2}}$. $[\boldsymbol{k}] = 1/\sqrt{3}(-1,-1,-1)^\top$.

Point group	Irreducible integrity basis
$\mathcal{T}, \mathcal{T}_h, \mathcal{O}, \mathcal{T}_d, \mathcal{O}_h$	$K_1 = C_{11} + C_{22} + C_{33}$ $\quad K_2 = C_{11}C_{22} + C_{22}C_{33} + C_{33}C_{11}$ $\quad K_3 = C_{11}C_{22}C_{33}$ $\quad K_4 = C_{23}^2 + C_{13}^2 + C_{12}^2$ $K_5 = C_{23}^2C_{13}^2 + C_{13}^2C_{12}^2 + C_{12}^2C_{23}^2$ $\quad K_6 = C_{12}C_{13}C_{23}$ $\quad L_1 = C_{11}\left(C_{13}^2 + C_{12}^2\right) + C_{22}\left(C_{12}^2 + C_{23}^2\right) + C_{33}\left(C_{23}^2 + C_{13}^2\right)$ $L_2 = C_{11}C_{13}^2C_{12}^2 + C_{22}C_{12}^2C_{23}^2 + C_{33}C_{23}^2C_{13}^2$ $\quad L_3 = C_{23}^2C_{22}C_{33} + C_{13}^2C_{33}C_{11} + C_{12}^2C_{11}C_{22}$
$\mathcal{T}, \mathcal{T}_h$	$L_4 = C_{11}\left(C_{13}^2 - C_{12}^2\right) + C_{22}\left(C_{12}^2 - C_{23}^2\right) + C_{33}\left(C_{23}^2 - C_{13}^2\right)$ $L_5 = C_{11}C_{22}\left(C_{11} - C_{22}\right) + C_{22}C_{33}\left(C_{22} - C_{33}\right) + C_{33}C_{11}\left(C_{33} - C_{11}\right)$ $L_6 = C_{23}^2C_{13}^2\left(C_{23}^2 - C_{13}^2\right) + C_{13}^2C_{12}^2\left(C_{13}^2 - C_{12}^2\right) + C_{12}^2C_{23}^2\left(C_{12}^2 - C_{23}^2\right)$ $L_7 = C_{11}C_{22}\left(C_{13}^2 - C_{23}^2\right) + C_{22}C_{33}\left(C_{12}^2 - C_{13}^2\right) + C_{33}C_{11}\left(C_{23}^2 - C_{12}^2\right)$ $L_8 = C_{23}^2C_{13}^2\left(C_{22} - C_{11}\right) + C_{13}^2C_{12}^2\left(C_{33} - C_{22}\right) + C_{12}^2C_{23}^2\left(C_{11} - C_{33}\right)$

Table 21: Polynomial relations between invariants of Tab. 10 and those proposed by Smith (1962) of group C_i. $[\boldsymbol{a}_1] = (0,0,1)^\top$ and $[\boldsymbol{a}_2] = (1,0,0)^\top$.

$K_1 = I_3 + I_1$ $\quad K_2 = -I_3 - I_2 - I_1$ $\quad K_3 = I_2 + I_1$ $\quad K_4 = -I_5$ $\quad K_5 = I_4$ $\quad K_6 = -I_6$
$I_1 = K_3 + K_2 + K_1$ $\quad I_2 = -K_2 - K_1$ $\quad I_3 = -K_3 - K_2$ $\quad I_4 = K_5$ $\quad I_5 = -K_4$ $\quad I_6 = -K_6$

Table 22: Polynomial relations between invariants of Tab. 10 and those proposed by Smith (1962) of group C_{1h}. $[\boldsymbol{a}_3] = (1,0,0)^\top$, $[\boldsymbol{a}_1] = (0,1,0)^\top$ and $[\boldsymbol{a}_2] = (0,0,1)^\top$.

$K_1 = -I_3 - I_2 + I_1$ $\quad K_2 = I_2$ $\quad K_3 = I_3$ $\quad K_4 = I_4$ $\quad K_5 = I_7 - I_4^2 - I_3^2$ $\quad 2K_6 = -2I_7 + I_5 - 2I_2I_3 - 2I_2^2 + 2I_1I_3 + 2I_1I_2 - I_1^2$ $L_1 = I_6 - I_3I_4 - I_2I_4$
$I_1 = K_3 + K_2 + K_1$ $\quad I_2 = K_2$ $\quad I_3 = K_3$ $\quad I_4 = K_4$ $\quad I_5 = 2K_6 + 2K_5 + 2K_4^2 + K_3^2 + K_2^2 + K_1^2$ $\quad I_6 = L_1 + K_3K_4 + K_2K_4$ $I_7 = K_5 + K_4^2 + K_3^2$

Table 23: Polynomial relations between invariants of Tab. 10 and those proposed by Smith (1962) of group C_{2h}. $[\boldsymbol{a}_3] = (1,0,0)^\top$, $[\boldsymbol{a}_1] = (0,1,0)^\top$ and $[\boldsymbol{a}_2] = (0,0,1)^\top$.

$K_1 = I_2 + I_1$ $\quad 2K_2 = I_3 - I_2$ $\quad 2K_3 = -I_3 - I_2$ $\quad 2K_4 = I_4$ $\quad 8K_5 = -4I_6 + 2I_5 - I_4^2 - I_3^2 - 4I_2I_3 - 3I_2^2 - 4I_1I_2 - 2I_1^2$ $8K_6 = 4I_6 + 2I_5 - I_4^2 - I_3^2 + 4I_2I_3 - 3I_2^2 - 4I_1I_2 - 2I_1^2$ $\quad 2L_1 = I_7 + I_2I_4$
$I_1 = K_3 + K_2 + K_1$ $\quad I_2 = -K_3 - K_2$ $\quad I_3 = -K_3 + K_2$ $\quad I_4 = 2K_4$ $\quad I_5 = 2K_6 + 2K_5 + 2K_4^2 + K_3^2 + K_2^2 + K_1^2$ $I_6 = K_6 - K_5 - K_3^2 + K_2^2$ $\quad I_7 = 2L_1 + 2K_3K_4 + 2K_2K_4$

Table 24: Polynomial relations between invariants of Tab. 10 and those proposed by Smith (1962) of groups C_{2v} and $\mathcal{D}_{2h}$. $[\boldsymbol{a}_1] = (0,0,1)^\top$ and $[\boldsymbol{a}_2] = (1,0,0)^\top$.

$2K_1 = I_3 - I_2$ $\quad K_2 = -I_3 + I_1$ $\quad 2K_3 = I_3 + I_2$ $\quad 2K_4 = -I_6 + I_5 + I_4 - I_3^2 - I_2I_3 + 2I_1I_3 - I_1^2$ $4K_5 = 4I_6 - 2I_4 + I_3^2 - I_2^2 - 4I_1I_3 + 2I_1^2$ $\quad 2K_6 = -I_6 - I_5 + I_4 - I_3^2 + I_2I_3 + 2I_1I_3 - I_1^2$ $12L_1 = 2I_7 - 9I_3I_6 + 6I_3I_4 - 3I_3^3 - 3I_2I_5 + 3I_2^2I_3 + 6I_1I_6 - 6I_1I_4 + 12I_1I_3^2 - 12I_1^2I_3 + 4I_1^3$
$I_1 = K_3 + K_2 + K_1$ $\quad I_2 = K_3 - K_1$ $\quad I_3 = K_3 + K_1$ $\quad I_4 = 2K_6 + 2K_5 + 2K_4 + K_3^2 + K_2^2 + K_1^2$ $\quad I_5 = -K_6 + K_4 + K_3^2 - K_1^2$ $I_6 = K_6 + 2K_5 + K_4 + K_3^2 + K_1^2$ $\quad I_7 = 6L_1 + 3K_3K_5 + 3K_3K_4 + K_3^3 + 3K_2K_6 + 3K_2K_4 + K_2^3 + 3K_1K_6 + 3K_1K_5 + K_1^3$

Table 25: Polynomial relations between invariants of Tab. 10 and those proposed by Smith (1962) of group $\mathcal{C}_{2i}$. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{a}_1] = (1,0,0)^\top$ and $[\boldsymbol{a}_2] = (0,1,0)^\top$.

$$K_1 = I_2 \qquad 4K_2 = I_4 - 2I_3 + 4I_2^2 - 4I_1I_2 + 2I_1^2 \qquad K_3 = -I_2 + I_1 \qquad K_4 = I_5 + I_3 - I_2^2 + 2I_1I_2 - I_1^2$$
$$\begin{aligned}192K_5 = &- 480I_1^3I_2 + 128I_1^4 + 654I_1^2I_2^2 - 288I_1^2I_3 + 30I_1^2I_4 - 312I_1^2I_5 - 384I_1I_2^3 + 540I_1I_2I_3 - 51I_1I_2I_4 + 576I_1I_2I_5 - 8I_1I_7\\ &- 6I_1I_9 + 12I_{11} + 84I_2^4 - 234I_2^2I_3 + 21I_2^2I_4 - 240I_2^2I_5 + 12I_2I_7 - 3I_2I_9 + 168I_3^2 - 36I_3I_4 + 360I_3I_5 - 36I_4I_5 + 192I_5^2\end{aligned}$$
$$4K_6 = -4I_5 + I_4 - 4I_3 + 4I_2^2 - 8I_1I_2 + 4I_1^2 \qquad 96L_1 = 3I_9 + 4I_7 + 3I_2I_4 - 6I_2I_3 + 12I_2^3 - 3I_1I_4 - 24I_1I_2^2 + 18I_1^2I_2 - 4I_1^3$$
$$16L_2 = -4I_7 + I_9 - 16I_2I_5 + I_2I_4 - 10I_2I_3 + 4I_2^3 + 16I_1I_5 - I_1I_4 + 16I_1I_3 - 24I_1I_2^2 + 30I_1^2I_2 - 12I_1^3 \qquad L_3 = I_6$$
$$12L_4 = I_{10} + 4I_8 \qquad 12L_5 = I_{10} - 8I_8 \qquad 48L_6 = 6I_{12} - 12I_5I_6 - 12I_3I_6 - 3I_2I_{10} + 12I_2I_8 + 12I_2^2I_6 - 2I_1I_{10} - 8I_1I_8 - 24I_1I_2I_6 + 12I_1^2I_6$$

$$I_1 = K_3 + K_1 \qquad I_2 = K_1 \qquad I_3 = 2K_6 + 2K_4 - 2K_2 + K_3^2 + K_1^2 \qquad I_4 = 4K_6 + 4K_4 \qquad I_5 = -2K_6 - K_4 + 2K_2 - K_1^2$$
$$I_6 = L_3 \qquad I_7 = -3L_2 + 6L_1 + 3K_3K_4 + K_3^3 + 3K_1K_6 + 3K_1K_4 - 3K_1K_2 + K_1^3 \qquad I_8 = -L_5 + L_4$$
$$I_9 = 4L_2 + 24L_1 + 4K_3K_6 \qquad I_{10} = 4L_5 + 8L_4 \qquad I_{11} = 16K_5 + 16K_4K_6 - 4K_2K_4 + 16K_3L_1 + 4K_3^2K_6 + 4K_1L_2 + 16K_1L_1$$
$$I_{12} = 8L_6 + 2K_4L_3 + 4K_3L_4 + 4K_1L_5 + 6K_1L_4$$

Table 26: Polynomial relations between invariants of Tab. 10 and those proposed by Smith (1962) of group $\mathcal{C}_{4h}$. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{a}_1] = (1,0,0)^\top$ and $[\boldsymbol{a}_2] = (0,1,0)^\top$.

$$K_1 = I_2 \qquad 2K_2 = -I_4 + I_2^2 \qquad K_3 = -I_2 + I_1 \qquad K_4 = -I_5 + I_3 - I_2^2 + 2I_1I_2 - I_1^2$$
$$\begin{aligned}68K_5 = &- 34I_{11} - 12I_6^2 + 34I_5^2 + 24I_4I_5 - 12I_4^2 - 34I_3I_5 - 12I_3I_4 + 17I_3^2 + 68I_2I_9 - 12I_2^2I_5 - 16I_2^2I_4 - 28I_2^2I_3\\ &+ 28I_2^4 - 68I_1I_2I_5 - 24I_1I_2I_4 + 68I_1I_2I_3 - 56I_1I_2^3 + 34I_1^2I_5 + 12I_1^2I_4 - 34I_1^2I_3 + 96I_1^2I_2^2 - 68I_1^3I_2 + 17I_1^4\end{aligned}$$
$$2K_6 = 2I_5 - I_4 - I_3 + I_2^2 - 2I_1I_2 + I_1^2 \qquad 6L_1 = -3I_9 + I_7 - 3I_2I_5 + 3I_2I_4 + 3I_2I_3 - 3I_2^3 + 3I_1I_5 - 3I_1I_3 + 6I_1I_2^2 - 6I_1^2I_2 + 2I_1^3$$
$$2L_2 = -2I_9 + 2I_2I_4 + I_2I_3 - 2I_2^3 + 2I_1I_2^2 - I_1^2I_2 \qquad L_3 = I_6 \qquad L_4 = I_{10} + I_8 - I_2I_6 \qquad L_5 = I_{10} - I_2I_6 \qquad L_6 = I_{12} - 2I_2I_{10} - I_2I_8 + I_2^2I_6$$

$$I_1 = K_3 + K_1 \qquad I_2 = K_1 \qquad I_3 = 2K_6 + 2K_4 - 2K_2 + K_3^2 + K_1^2 \qquad I_4 = -2K_2 + K_1^2 \qquad I_5 = 2K_6 + K_4 - 2K_2 + K_1^2 \qquad I_6 = L_3$$
$$I_7 = -3L_2 + 6L_1 + 3K_3K_4 + K_3^3 + 3K_1K_6 + 3K_1K_4 - 3K_1K_2 + K_1^3 \qquad I_8 = -L_5 + L_4 \qquad I_9 = -L_2 + K_1K_6 + K_1K_4 - 3K_1K_2 + K_1^3$$
$$I_{10} = L_5 + K_1L_3 \qquad I_{11} = -2K_5 + L_3^2 + 2K_6^2 + 2K_4K_6 + K_4^2 - 2K_2K_4 + 2K_2^2 - 2K_1L_2 + K_1^2K_6 + 2K_1^2K_4 - 4K_1^2K_2 + K_1^4$$
$$I_{12} = L_6 + K_1L_5 + K_1L_4 + K_1^2L_3$$

Table 27: Polynomial relations between invariants of Tab. 10 and those proposed by Smith (1962) of groups $\mathcal{C}_{4v}$ and $\mathcal{D}_{4h}$. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{a}_1] = (1,0,0)^\top$ and $[\boldsymbol{a}_2] = (0,1,0)^\top$.

$$K_1 = I_2 \qquad 2K_2 = -I_4 + I_2^2 \qquad K_3 = -I_2 + I_1 \qquad K_4 = -I_5 + I_3 - I_2^2 + 2I_1I_2 - I_1^2$$
$$4K_5 = -2I_8 + 2I_5^2 - 2I_3I_5 + I_3^2 + 4I_2I_7 - 2I_2^2I_4 - 2I_2^2I_3 + 2I_2^4 - 4I_1I_2I_5 + 4I_1I_2I_3 - 4I_1I_2^3 + 2I_1^2I_5 - 2I_1^2I_3 + 6I_1^2I_2^2 - 4I_1^3I_2 + I_1^4$$
$$2K_6 = 2I_5 - I_4 - I_3 + I_2^2 - 2I_1I_2 + I_1^2 \qquad 6L_1 = -3I_7 + I_6 - 3I_2I_5 + 3I_2I_4 + 3I_2I_3 - 3I_2^3 + 3I_1I_5 - 3I_1I_3 + 6I_1I_2^2 - 6I_1^2I_2 + 2I_1^3$$
$$2L_2 = -2I_7 + 2I_2I_4 + I_2I_3 - 2I_2^3 + 2I_1I_2^2 - I_1^2I_2$$

$$I_1 = K_3 + K_1 \qquad I_2 = K_1 \qquad I_3 = 2K_6 + 2K_4 - 2K_2 + K_3^2 + K_1^2 \qquad I_4 = -2K_2 + K_1^2 \qquad I_5 = 2K_6 + K_4 - 2K_2 + K_1^2$$
$$I_6 = -3L_2 + 6L_1 + 3K_3K_4 + K_3^3 + 3K_1K_6 + 3K_1K_4 - 3K_1K_2 + K_1^3 \qquad I_7 = -L_2 + K_1K_6 + K_1K_4 - 3K_1K_2 + K_1^3$$
$$I_8 = -2K_5 + 2K_6^2 + 2K_4K_6 + K_4^2 - 4K_2K_6 - 2K_2K_4 + 2K_2^2 - 2K_1L_2 + 2K_1^2K_6 + 2K_1^2K_4 - 4K_1^2K_2 + K_1^4$$

Table 28: Polynomial relations between invariants of Tab. 10 and those proposed by Smith (1962) of group $\mathcal{D}_{2d}$. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{a}_1] = (1,0,0)^\top$ and $[\boldsymbol{a}_2] = (0,1,0)^\top$.

$$K_1 = I_2 \quad 4K_2 = I_4 - 2I_3 + 4I_2^2 - 4I_1I_2 + 2I_1^2 \quad K_3 = -I_2 + I_1 \quad K_4 = I_5 - I_2^2 + 2I_1I_2 - I_1^2$$
$$192K_5 = -36I_4I_5 + 12I_8 + 192I_5^2 - 24I_3I_5 - 3I_2I_7 + 12I_2I_6 - 240I_2^2I_5 + 21I_2^2I_4 + 6I_2^2I_3 + 84I_2^4 - 6I_1I_7 - 8I_1I_6 + 576I_1I_2I_5$$
$$- 51I_1I_2I_4 - 36I_1I_2I_3 - 384I_1I_2^3 - 312I_1^2I_5 + 30I_1^2I_4 + 24I_1^2I_3 + 654I_1^2I_2^2 - 480I_1^3I_2 + 128I_1^4$$
$$4K_6 = -4I_5 + I_4 + 4I_2^2 - 8I_1I_2 + 4I_1^2 \quad 96L_1 = 3I_7 + 4I_6 + 3I_2I_4 - 6I_2I_3 + 12I_2^3 - 3I_1I_4 - 24I_1I_2^2 + 18I_1^2I_2 - 4I_1^3$$
$$16L_2 = I_7 - 4I_6 - 16I_2I_5 + I_2I_4 + 6I_2I_3 + 4I_2^3 + 16I_1I_5 - I_1I_4 - 24I_1I_2^2 + 30I_1^2I_2 - 12I_1^3$$

$$I_1 = K_3 + K_1 \quad I_2 = K_1 \quad I_3 = 2K_6 + 2K_4 - 2K_2 + K_3^2 + K_1^2 \quad I_4 = 4K_6 + 4K_4 \quad I_5 = K_4 + K_3^2$$
$$I_6 = -3L_2 + 6L_1 + 3K_3K_4 + K_3^3 + 3K_1K_6 + 3K_1K_4 - 3K_1K_2 + K_1^3 \quad I_7 = 4L_2 + 24L_1 + 4K_3K_6$$
$$I_8 = 16K_5 + 16K_4K_6 - 4K_2K_4 + 16K_3L_1 + 4K_3^2K_6 + 4K_1L_2 + 16K_1L_1$$

Table 29: Polynomial relations between invariants of Tab. 11 and those proposed by Smith (1962) of group $\mathcal{C}_{3i}$. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{l}_1] = (1,0,0)^\top$, $[\boldsymbol{l}_2] = \left(-1/2, \sqrt{3}/2, 0\right)^\top$ and $[\boldsymbol{l}_3] = \left(-1/2, -\sqrt{3}/2, 0\right)^\top$.

$$K_1 = -I_2 \quad 36K_2 = -32I_4 + 9I_2^2 \quad 9K_3 = 64I_{10} + 32I_2I_4 - 18I_2^3 - 32I_1I_4 \quad K_4 = I_2 + I_1$$
$$36K_5 = -32I_4 + 18I_3 - 27I_2^2 - 36I_1I_2 - 18I_1^2 \quad 3K_6 = -8I_{14} - 8I_2I_6 \quad 3L_1 = 8I_6$$
$$36L_2 = 12I_7 + 64I_2I_4 - 18I_2I_3 + 18I_2^3 + 32I_1I_4 - 18I_1I_3 + 27I_1I_2^2 + 18I_1^2I_2 + 6I_1^3 \quad 3L_3 = 16I_{12} - 24I_2I_6 - 16I_1I_6$$
$$3L_4 = 4I_5 \quad 9L_5 = 64I_{13} \quad 3L_6 = 4I_{11} + 4I_2I_5 \quad 3L_7 = -8I_9 - 4I_2I_5 + 8I_1I_5 \quad L_8 = -I_8$$

$$I_1 = K_4 + K_1 \quad I_2 = -K_1 \quad I_3 = 2K_5 - 2K_2 + K_4^2 + K_1^2 \quad 32I_4 = -36K_2 + 9K_1^2 \quad 4I_5 = 3L_4 \quad 8I_6 = 3L_1$$
$$I_7 = 3L_2 + 3K_4K_5 + K_4^3 - 3K_1K_2 + K_1^3 \quad I_8 = -L_8 \quad 8I_9 = -3L_7 + 6K_4L_4 + 9K_1L_4 \quad 64I_{10} = 9K_3 - 36K_4K_2 - 72K_1K_2 + 9K_1^2K_4$$
$$4I_{11} = 3L_6 + 3K_1L_4 \quad 16I_{12} = 3L_3 + 6K_4L_1 - 3K_1L_1 \quad 64I_{13} = 9L_5 \quad 8I_{14} = -3K_6 + 3K_1L_1$$

Table 30: Polynomial relations between invariants of Tab. 11 and those proposed by Smith (1962) of group $\mathcal{C}_{3v}$. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{l}_1] = (1,0,0)^\top$, $[\boldsymbol{l}_2] = \left(-1/2, \sqrt{3}/2, 0\right)^\top$ and $[\boldsymbol{l}_3] = \left(-1/2, -\sqrt{3}/2, 0\right)^\top$.

$$K_1 = -I_2 + I_1 \quad 36K_2 = 8I_4 + 9I_2^2 - 18I_1I_2 + 9I_1^2 \quad 9K_3 = 16I_7 - 16I_2I_4 - 18I_2^3 + 8I_1I_4 + 54I_1I_2^2 - 54I_1^2I_2 + 18I_1^3$$
$$K_4 = I_2 \quad 36K_5 = 8I_4 + 18I_3 - 27I_2^2 + 18I_1I_2 - 9I_1^2 \quad 3K_6 = -4I_9 - 4I_2I_5 + 4I_1I_5 \quad 3L_1 = 4I_5$$
$$36L_2 = 12I_6 - 16I_2I_4 - 18I_2I_3 + 18I_2^3 + 8I_1I_4 - 27I_1I_2^2 + 18I_1^2I_2 - 3I_1^3 \quad 3L_3 = 8I_8 - 12I_2I_5 + 4I_1I_5$$

$$I_1 = K_4 + K_1 \quad I_2 = K_4 \quad I_3 = 2K_5 - 2K_2 + K_4^2 + K_1^2 \quad 8I_4 = 36K_2 - 9K_1^2 \quad 4I_5 = 3L_1 \quad I_6 = 3L_2 + 3K_4K_5 + K_4^3 - 3K_1K_2 + K_1^3$$
$$16I_7 = 9K_3 + 36K_4K_2 - 36K_1K_2 - 9K_1^2K_4 - 9K_1^3 \quad 8I_8 = 3L_3 + 6K_4L_1 - 3K_1L_1 \quad 4I_9 = -3K_6 + 3K_1L_1$$

Table 31: Polynomial relations between invariants of Tab. 11 and those proposed by Smith (1962) of group $\mathcal{D}_{3d}$. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{l}_1] = (1,0,0)^\top$, $[\boldsymbol{l}_2] = \left(-1/2, \sqrt{3}/2, 0\right)^\top$ and $[\boldsymbol{l}_3] = \left(-1/2, -\sqrt{3}/2, 0\right)^\top$.

$$K_1 = -I_2 + I_1 \quad 36K_2 = 8I_4 + 9I_2^2 - 18I_1I_2 + 9I_1^2 \quad 9K_3 = 16I_7 - 16I_2I_4 - 18I_2^3 + 8I_1I_4 + 54I_1I_2^2 - 54I_1^2I_2 + 18I_1^3 \quad K_4 = I_2$$
$$36K_5 = 8I_4 + 18I_3 - 27I_2^2 + 18I_1I_2 - 9I_1^2 \quad 3K_6 = 4I_9 + 4I_2I_5 - 4I_1I_5 \quad 3L_1 = -4I_5$$
$$36L_2 = 12I_6 - 16I_2I_4 - 18I_2I_3 + 18I_2^3 + 8I_1I_4 - 27I_1I_2^2 + 18I_1^2I_2 - 3I_1^3 \quad 3L_3 = -8I_8 + 12I_2I_5 - 4I_1I_5$$

$$I_1 = K_4 + K_1 \quad I_2 = K_4 \quad I_3 = 2K_5 - 2K_2 + K_4^2 + K_1^2 \quad 8I_4 = 36K_2 - 9K_1^2 \quad 4I_5 = -3L_1 \quad I_6 = 3L_2 + 3K_4K_5 + K_4^3 - 3K_1K_2 + K_1^3$$
$$16I_7 = 9K_3 + 36K_4K_2 - 36K_1K_2 - 9K_1^2K_4 - 9K_1^3 \quad 8I_8 = -3L_3 - 6K_4L_1 + 3K_1L_1 \quad 4I_9 = 3K_6 - 3K_1L_1$$

Table 32: Polynomial relations between invariants of Tab. 11 and those proposed by Smith (1962) of group C_{3h}. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{l}_1] = (1,0,0)^\top$, $[\boldsymbol{l}_2] = \left(-1/2, \sqrt{3}/2, 0\right)^\top$ and $[\boldsymbol{l}_3] = \left(-1/2, -\sqrt{3}/2, 0\right)^\top$.

$K_1 = -I_2 \qquad 36K_2 = -16I_4 + 9I_2^2 \qquad 9K_3 = 16I_7 + 32I_2I_4 - 18I_2^3 \qquad 36K_4 = -16I_4 + 18I_3 - 27I_2^2 - 36I_1I_2 - 18I_1^2 \qquad K_5 = I_2 + I_1$

$$\begin{aligned}46656K_6 = &- 4096I_4^3 + 82944I_{13} + 9216I_3I_4^2 - 5184I_3^2I_4 + 248832I_2I_{11} + 13824I_2I_4I_5 + 15552I_2I_3I_5 + 248832I_2^2I_9 - 48384I_2^2I_4^2 \\ &- 72576I_2^2I_3I_4 + 2916I_2^2I_3^2 + 82944I_2^3I_7 - 101088I_2^3I_5 + 37584I_2^4I_4 + 37908I_2^4I_3 - 5103I_2^6 + 20736I_1I_2I_3I_4 \\ &- 23328I_1I_2I_3^2 - 31104I_1I_2^2I_5 + 128304I_1I_2^3I_3 - 9216I_1^2I_4^2 + 10368I_1^2I_3I_4 - 15552I_1^2I_2I_5 + 10368I_1^2I_2^2I_4 + 40824I_1^2I_2^2I_3 \\ &- 2916I_1^2I_2^4 - 34560I_1^3I_2I_4 + 31104I_1^3I_2I_3 - 27216I_1^3I_2^3 - 5184I_1^4I_4 - 12636I_1^4I_2^2 - 7776I_1^5I_2\end{aligned}$$

$36L_1 = -12I_5 - 16I_2I_4 + 9I_2^3 - 16I_1I_4 + 18I_1I_3 + 9I_1I_2^2 - 6I_1^3$

$$\begin{aligned}648L_2 = &- 216I_3I_5 + 1152I_{11} + 192I_4I_5 + 2304I_2I_9 - 256I_2I_4^2 - 864I_2I_3I_4 + 1152I_2^2I_7 - 108I_2^2I_5 + 864I_2^3I_4 + 486I_2^3I_3 - 405I_2^5 \\ &+ 256I_1I_4^2 - 576I_1I_3I_4 + 324I_1I_3^2 + 432I_1I_2I_5 + 1440I_1I_2^2I_4 + 324I_1I_2^2I_3 - 891I_1I_2^4 + 216I_1^2I_5 + 1440I_1^2I_2I_4 \\ &- 648I_1^2I_2I_3 - 810I_1^2I_2^3 + 384I_1^3I_4 - 432I_1^3I_3 - 216I_1^3I_2^2 + 216I_1^4I_2 + 108I_1^5\end{aligned}$$

$36L_3 = -64I_9 + 32I_3I_4 - 64I_2I_7 - 24I_2I_5 - 80I_2^2I_4 - 18I_2^2I_3 + 45I_2^4 - 96I_1I_2I_4 + 36I_1I_2I_3 + 54I_1I_2^3 - 32I_1^2I_4 + 18I_1^2I_2^2 - 12I_1^3I_2$

$L_4 = I_6 \qquad 9L_5 = -16I_8$

$$\begin{aligned}44775L_6 = &- 79600I_{14} + 3456I_6I_7 + 1152I_5I_8 - 3072I_4I_{10} - 238800I_2I_{12} - 768I_2I_4I_8 + 1728I_2I_4I_6 - 864I_2I_3I_8 - 238800I_2^2I_{10} \\ &- 79168I_2^3I_8 + 1536I_1I_4I_8 - 1728I_1I_3I_8 + 864I_1I_2^2I_8 + 864I_1^2I_2I_8 + 576I_1^3I_8\end{aligned}$$

$9L_7 = 16I_{10} + 16I_2I_8 + 18I_2I_6 \qquad 18L_8 = 32I_{12} - 16I_4I_6 + 18I_3I_6 + 64I_2I_{10} + 32I_2^2I_8 - 27I_2^2I_6 - 36I_1I_2I_6 - 18I_1^2I_6$

$I_1 = K_5 + K_1 \qquad I_2 = -K_1 \qquad I_3 = 2K_4 - 2K_2 + K_5^2 + K_1^2 \qquad 16I_4 = -36K_2 + 9K_1^2 \qquad I_5 = -3L_1 + 3K_5K_4 + K_5^3 + 3K_1K_4 - 3K_1K_2 + K_1^3$

$I_6 = L_4 \qquad 16I_7 = 9K_3 - 72K_1K_2 \qquad 16I_8 = -9L_5 \qquad 16I_9 = -9L_3 - 36K_2K_4 + 36K_2^2 - 18K_1L_1 + 9K_1K_3 - 81K_1^2K_2$

$16I_{10} = 9L_7 - 9K_1L_5 + 18K_1L_4 \qquad 16I_{11} = 9L_2 - 18K_4L_1 - 18K_1L_3 - 36K_1K_2K_4 - 54K_1^2L_1 + 9K_1^2K_3 - 72K_1^3K_2$

$16I_{12} = 9L_8 - 18K_4L_4 + 18K_1L_7 - 9K_1^2L_5 + 36K_1^2L_4$

$16I_{13} = -9K_2K_4^2 + 9K_6 + 27K_1L_2 - 72K_1K_4L_1 + 36K_1K_2L_1 - 27K_1^2L_3 - 90K_1^2K_2K_4 + 36K_1^2K_2^2 - 72K_1^3L_1 + 9K_1^3K_3 - 81K_1^4K_2$

$$\begin{aligned}272I_{14} = &- 153L_6 + 126L_1L_5 + 126K_3L_4 + 252K_2L_7 + 459K_1L_8 - 63K_1K_4L_5 - 918K_1K_4L_4 - 252K_1K_2L_4 + 396K_1^2L_7 \\ &- 153K_1^3L_5 + 729K_1^3L_4\end{aligned}$$

Table 33: Polynomial relations between invariants of Tab. 11 and those proposed by Smith (1962) of group C_{6h}. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{l}_1] = (1,0,0)^\top$, $[\boldsymbol{l}_2] = \left(-1/2, \sqrt{3}/2, 0\right)^\top$ and $[\boldsymbol{l}_3] = \left(-1/2, -\sqrt{3}/2, 0\right)^\top$.

$$K_1 = -I_2 \qquad 12K_2 = -8I_4 + 9I_2^2 \qquad 3K_3 = 16I_7 + 36I_2I_4 - 27I_2^3 \qquad 12K_4 = -8I_4 + 6I_3 - 3I_2^2 - 12I_1I_2 - 6I_1^2 \qquad K_5 = I_2 + I_1$$

$$\begin{aligned}3456K_6 = &- 5632I_4^3 + 18432I_{13} - 1152I_3I_4^2 - 2592I_3^2I_4 - 1944I_3^3 + 55296I_2I_{11} + 55296I_2^2I_9 + 21312I_2^2I_4^2 + 12960I_2^2I_3I_4 \\ &+ 14580I_2^2I_3^2 + 18432I_2^3I_7 - 36936I_2^4I_4 - 36450I_2^4I_3 + 38151I_2^6 + 2304I_1I_2I_4^2 + 10368I_1I_2I_3I_4 + 11664I_1I_2I_3^2 \\ &- 25920I_1I_2^3I_4 - 58320I_1I_2^3I_3 + 72900I_1I_2^5 + 1152I_1^2I_4^2 + 5184I_1^2I_3I_4 + 5832I_1^2I_3^2 - 23328I_1^2I_2^2I_4 - 52488I_1^2I_2^2I_3 \\ &+ 94770I_1^2I_2^4 - 10368I_1^3I_2I_4 - 23328I_1^3I_2I_3 + 73872I_1^3I_2^3 - 2592I_1^4I_4 - 5832I_1^4I_3 + 37908I_1^4I_2^2 + 11664I_1^5I_2 + 1944I_1^6\end{aligned}$$

$$12L_1 = -4I_5 - 8I_2I_4 + 9I_2^3 - 8I_1I_4 + 6I_1I_3 + 9I_1I_2^2 - 2I_1^3$$

$$\begin{aligned}288L_2 = &- 128I_4I_5 + 1536I_{11} - 288I_3I_5 + 3072I_2I_9 - 192I_2I_4^2 - 288I_2I_3I_4 + 324I_2I_3^2 + 1536I_2^2I_7 + 720I_2^2I_5 + 1008I_2^3I_4 - 972I_2^3I_3 \\ &+ 405I_2^5 - 256I_1I_4^2 - 384I_1I_3I_4 + 432I_1I_3^2 + 576I_1I_2I_5 + 2304I_1I_2^2I_4 - 1728I_1I_2^2I_3 + 324I_1I_2^4 + 288I_1^2I_5 + 1440I_1^2I_2I_4 \\ &- 1512I_1^2I_2I_3 + 972I_1^2I_2^3 + 512I_1^3I_4 - 576I_1^3I_3 + 1008I_1^3I_2^2 + 612I_1^4I_2 + 144I_1^5\end{aligned}$$

$$18L_3 = -96I_9 + 16I_4^2 + 36I_3I_4 - 96I_2I_7 - 36I_2I_5 - 162I_2^2I_4 + 81I_2^4 - 144I_1I_2I_4 + 54I_1I_2I_3 + 81I_1I_2^3 - 36I_1^2I_4 - 18I_1^3I_2$$

$$L_4 = I_6 \qquad 3L_5 = 16I_8$$

$$\begin{aligned}9159L_6 = &- 12672I_5I_8 + 48848I_{14} + 38016I_6I_7 + 50688I_4I_{10} + 146544I_2I_{12} + 12672I_2I_4I_8 - 54264I_2I_4I_6 + 9504I_2I_3I_8 \\ &- 54954I_2I_3I_6 + 108528I_2^2I_{10} + 34592I_2^3I_8 - 27477I_2^3I_6 - 25344I_1I_4I_8 + 19008I_1I_3I_8 + 9504I_1I_2^2I_8 \\ &+ 109908I_1I_2^2I_6 - 9504I_1^2I_2I_8 + 54954I_1^2I_2I_6 - 6336I_1^3I_8\end{aligned}$$

$$3L_7 = -16I_{10} - 16I_2I_8 + 18I_2I_6 \qquad 6L_8 = -32I_{12} + 8I_4I_6 + 18I_3I_6 - 64I_2I_{10} - 32I_2^2I_8 + 27I_2^2I_6 - 36I_1I_2I_6 - 18I_1^2I_6$$

$$I_1 = K_5 + K_1 \qquad I_2 = -K_1 \qquad I_3 = 2K_4 - 2K_2 + K_5^2 + K_1^2 \qquad 8I_4 = -12K_2 + 9K_1^2 \qquad I_5 = -3L_1 + 3K_5K_4 + K_5^3 + 3K_1K_4 - 3K_1K_2 + K_1^3$$

$$I_6 = L_4 \qquad 32I_7 = 6K_3 - 108K_1K_2 + 27K_1^3 \qquad 16I_8 = 3L_5$$

$$32I_9 = -6L_3 - 36K_2K_4 + 48K_2^2 - 36K_1L_1 + 6K_1K_3 + 27K_1^2K_4 - 144K_1^2K_2 + 27K_1^4 \qquad 16I_{10} = -3L_7 + 3K_1L_5 - 18K_1L_4$$

$$32I_{11} = -36K_4L_1 + 6L_2 + 48K_2L_1 - 12K_1L_3 + 27K_1K_4^2 - 144K_1K_2K_4 + 144K_1K_2^2 - 72K_1^2L_1 + 6K_1^2K_3 + 54K_1^3K_4 - 180K_1^3K_2 + 27K_1^5$$

$$16I_{12} = -3L_8 + 18K_4L_4 - 24K_2L_4 - 6K_1L_7 + 3K_1^2L_5$$

$$\begin{aligned}32I_{13} = &- 108K_2K_4^2 + 6K_6 + 27K_4^3 + 144K_2^2K_4 - 96K_2^3 + 18K_1L_2 - 108K_1K_4L_1 + 144K_1K_2L_1 - 18K_1^2L_3 + 81K_1^2K_4^2 \\ &- 324K_1^2K_2K_4 + 288K_1^2K_2^2 - 108K_1^3L_1 + 6K_1^3K_3 + 81K_1^4K_4 - 216K_1^4K_2 + 27K_1^6\end{aligned}$$

$$272I_{14} = -42L_1L_5 + 51L_6 - 42K_3L_4 - 84K_2L_7 - 153K_1L_8 + 21K_1K_4L_5 + 306K_1K_4L_4 + 84K_1K_2L_4 - 132K_1^2L_7 + 51K_1^3L_5 - 243K_1^3L_4$$

Table 34: Polynomial relations between invariants of Tab. 11 and those proposed by Smith (1962) of group $\mathcal{T}_d$. $[\boldsymbol{a}_1] = (1,0,0)^\top$, $[\boldsymbol{a}_2] = (0,1,0)^\top$ and $[\boldsymbol{a}_3] = (0,0,1)^\top$.

$$K_1 = I_1 \qquad 4K_2 = I_3 - 2I_2 + 2I_1^2 \qquad 36K_3 = -8I_6 + I_5 + 12I_4 + 8I_1I_3 - 18I_1I_2 + 6I_1^3 \qquad 4K_4 = I_3$$

$$36K_5 = 3I_8 - 3I_7 + 4I_1I_6 - 2I_1I_5 - I_1^2I_3 \qquad 36K_6 = I_6 + I_5 - I_1I_3 \qquad 12L_1 = 2I_6 - I_5 + I_1I_3$$

$$72L_2 = 3 - I_3I_6 + 6I_9 - I_3I_5 - 2I_3I_4 + 4I_2I_6 + I_2I_5 - 6I_1I_8 + 12I_1I_7 + I_1I_3^2 - I_1I_2I_3 - 20I_1^2I_6 + I_1^2I_5 + 7I_1^3I_3$$

$$144L_3 = -12I_8 + 48I_7 + 9I_3^2 - 18I_2I_3 - 56I_1I_6 + 4I_1I_5 + 26I_1^2I_3$$

$$I_1 = K_1 \qquad I_2 = 2K_4 - 2K_2 + K_1^2 \qquad I_3 = 4K_4 \qquad I_4 = 3L_1 + 6K_6 + 3K_3 - 3K_1K_2 + K_1^3 \qquad I_5 = -4L_1 + 24K_6 + 4K_1K_4$$

$$I_6 = 4L_1 + 12K_6 \qquad I_7 = 4L_3 + 4K_5 - 4K_2K_4 + 4K_1L_1 + 16K_1K_6 \qquad I_8 = 4L_3 + 16K_5 - 4K_2K_4 - 4K_1L_1 + 16K_1K_6 + 4K_1^2K_4$$

$$I_9 = 12L_2 + 8K_4K_6 + 4K_4K_3 + 4K_2L_1 + 24K_2K_6 - 4K_1L_3 + 8K_1K_5 + 8K_1^2K_6$$

Table 35: Polynomial relations between invariants of Tab. 11 and those proposed by Smith (1962) of group $\mathcal{D}_{3h}$. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{l}_1] = (1,0,0)^\top$, $[\boldsymbol{l}_2] = \left(-1/2, \sqrt{3}/2, 0\right)^\top$ and $[\boldsymbol{l}_3] = \left(-1/2, -\sqrt{3}/2, 0\right)^\top$.

$$K_1 = -I_2 + I_1 \qquad 36K_2 = -16I_4 + 9I_2^2 - 18I_1I_2 + 9I_1^2 \qquad 9K_3 = 16I_6 + 32I_2I_4 - 18I_2^3 - 32I_1I_4 + 54I_1I_2^2 - 54I_1^2I_2 + 18I_1^3$$

$$36K_4 = -16I_4 + 18I_3 - 27I_2^2 + 18I_1I_2 - 9I_1^2 \qquad K_5 = I_2$$

$$\begin{aligned}46656K_6 = &-4096I_4^3 + 82944I_9 + 9216I_3I_4^2 - 5184I_3^2I_4 + 248832I_2I_8 + 13824I_2I_4I_5 + 15552I_2I_3I_5 + 248832I_2^2I_7 - 48384I_2^2I_4^2\\ &- 72576I_2^2I_3I_4 + 2916I_2^2I_3^2 + 82944I_2^3I_6 - 101088I_2^3I_5 + 37584I_2^4I_4 + 37908I_2^4I_3 - 5103I_2^6 - 248832I_1I_8\\ &- 13824I_1I_4I_5 - 15552I_1I_3I_5 - 497664I_1I_2I_7 + 96768I_1I_2I_4^2 + 165888I_1I_2I_3I_4 - 29160I_1I_2I_3^2 - 248832I_1I_2^2I_6\\ &+ 272160I_1I_2^2I_5 - 150336I_1I_2^3I_4 - 23328I_1I_2^3I_3 + 30618I_1I_2^5 + 248832I_1^2I_7 - 57600I_1^2I_4^2 - 82944I_1^2I_3I_4 + 26244I_1^2I_3^2\\ &+ 248832I_1^2I_2I_6 - 256608I_1^2I_2I_5 + 235872I_1^2I_2^2I_4 - 116640I_1^2I_2^2I_3 - 79461I_1^2I_2^4 - 82944I_1^3I_6 + 85536I_1^3I_5\\ &- 205632I_1^3I_2I_4 + 182736I_1^3I_2I_3 + 86508I_1^3I_2^3 + 77328I_1^4I_4 - 80676I_1^4I_3 - 25029I_1^4I_2^2 - 21870I_1^5I_2 + 14337I_1^6\end{aligned}$$

$$36L_1 = -12I_5 - 16I_2I_4 + 9I_2^3 + 18I_1I_3 - 18I_1I_2^2 + 9I_1^2I_2 - 6I_1^3$$

$$\begin{aligned}648L_2 = &-216I_3I_5 + 1152I_8 + 192I_4I_5 + 2304I_2I_7 - 256I_2I_4^2 - 864I_2I_3I_4 + 1152I_2^2I_6 - 108I_2^2I_5 + 864I_2^3I_4 + 486I_2^3I_3 - 405I_2^5\\ &- 2304I_1I_7 + 512I_1I_4^2 + 288I_1I_3I_4 + 324I_1I_3^2 - 2304I_1I_2I_6 + 648I_1I_2I_5 - 1152I_1I_2^2I_4 - 1134I_1I_2^2I_3 + 1134I_1I_2^4\\ &+ 1152I_1^2I_6 - 324I_1^2I_5 + 1152I_1^2I_2I_4 + 162I_1^2I_2I_3 - 1296I_1^2I_2^3 - 480I_1^3I_4 + 54I_1^3I_3 + 918I_1^3I_2^2 - 243I_1^4I_2\end{aligned}$$

$$\begin{aligned}36L_3 = &-64I_7 + 32I_3I_4 - 64I_2I_6 - 24I_2I_5 - 80I_2^2I_4 - 18I_2^2I_3 + 45I_2^4 + 64I_1I_6 + 24I_1I_5 + 64I_1I_2I_4 + 72I_1I_2I_3 - 126I_1I_2^3 - 16I_1^2I_4\\ &- 54I_1^2I_3 + 126I_1^2I_2^2 - 66I_1^3I_2 + 21I_1^4\end{aligned}$$

$$I_1 = K_5 + K_1 \qquad I_2 = K_5 \qquad I_3 = 2K_4 - 2K_2 + K_5^2 + K_1^2 \qquad 16I_4 = -36K_2 + 9K_1^2 \qquad I_5 = -3L_1 + 3K_5K_4 + K_5^3 + 3K_1K_4 - 3K_1K_2 + K_1^3$$

$$16I_6 = 9K_3 - 72K_1K_2 \qquad 16I_7 = -9L_3 - 36K_2K_4 + 36K_2^2 - 18K_1L_1 + 9K_1K_3 - 81K_1^2K_2$$

$$16I_8 = 9L_2 - 18K_4L_1 - 18K_1L_3 - 36K_1K_2K_4 - 54K_1^2L_1 + 9K_1^2K_3 - 72K_1^3K_2$$

$$16I_9 = -9K_2K_4^2 + 9K_6 + 27K_1L_2 - 72K_1K_4L_1 + 36K_1K_2L_1 - 27K_1^2L_3 - 90K_1^2K_2K_4 + 36K_1^2K_2^2 - 72K_1^3L_1 + 9K_1^3K_3 - 81K_1^4K_2$$

Table 36: Polynomial relations between invariants of Tab. 11 and those proposed by Smith (1962) of group $\mathcal{O}_h$. $[\boldsymbol{a}_1] = (1,0,0)^\top$, $[\boldsymbol{a}_2] = (0,1,0)^\top$ and $[\boldsymbol{a}_3] = (0,0,1)^\top$.

$$K_1 = I_1 \qquad 2K_2 = -I_3 + I_1^2 \qquad 6K_3 = 2I_5 - 3I_1I_3 + I_1^3 \qquad 2K_4 = -I_3 + I_2 \qquad 12K_5 = 12I_8 - 6I_7 - 6I_2I_3 + 3I_2^2 - 8I_1I_5 + 6I_1^2I_3 - I_1^4$$

$$6K_6 = -3I_6 + 2I_5 + I_4 \qquad L_1 = I_6 - I_5$$

$$12L_2 = -6I_3I_6 + 12I_9 + 4I_3I_5 - 6I_2I_6 - 2I_2I_5 - 12I_1I_8 - 6I_1I_7 + 6I_1I_2I_3 + 3I_1I_2^2 + 12I_1^2I_6 + 2I_1^2I_5 - 4I_1^3I_3 - 4I_1^3I_2 + I_1^5$$

$$12L_3 = -12I_8 + 3I_3^2 + 3I_2I_3 + 12I_1I_6 + 4I_1I_5 - 9I_1^2I_3 - 3I_1^2I_2 + 2I_1^4$$

$$I_1 = K_1 \qquad I_2 = 2K_4 - 2K_2 + K_1^2 \qquad I_3 = -2K_2 + K_1^2 \qquad I_4 = 3L_1 + 6K_6 + 3K_3 - 3K_1K_2 + K_1^3$$

$$I_5 = 3K_3 - 3K_1K_2 + K_1^3 \qquad I_6 = L_1 + 3K_3 - 3K_1K_2 + K_1^3 \qquad I_7 = -2L_3 - 2K_5 + 2K_4^2 - 2K_2K_4 + 2K_2^2 + 2K_1L_1 + 4K_1K_3 - 4K_1^2K_2 + K_1^4$$

$$I_8 = -L_3 - K_2K_4 + 2K_2^2 + K_1L_1 + 4K_1K_3 - 4K_1^2K_2 + K_1^4$$

$$I_9 = -2K_2L_1 + L_2 + K_4L_1 + 4K_4K_3 - 5K_2K_3 - 2K_1L_3 - K_1K_5 - 2K_1K_2K_4 + 5K_1K_2^2 + 2K_1^2L_1 + 5K_1^2K_3 - 5K_1^3K_2 + K_1^5$$

Table 37: Polynomial relations between invariants of Tab. 11 and those proposed by Smith (1962) of groups $\mathcal{C}_{6v}$ and $\mathcal{D}_{6h}$. $[\boldsymbol{a}_3] = (0,0,1)^\top$, $[\boldsymbol{l}_1] = (1,0,0)^\top$, $[\boldsymbol{l}_2] = \left(-1/2, \sqrt{3}/2, 0\right)^\top$ and $[\boldsymbol{l}_3] = \left(-1/2, -\sqrt{3}/2, 0\right)^\top$.

$K_1 = -I_2 + I_1 \qquad 12K_2 = -8I_4 + 9I_2^2 - 18I_1I_2 + 9I_1^2 \qquad 3K_3 = 16I_6 + 36I_2I_4 - 27I_2^3 - 36I_1I_4 + 81I_1I_2^2 - 81I_1^2I_2 + 27I_1^3$

$12K_4 = -8I_4 + 6I_3 - 3I_2^2 - 6I_1I_2 + 3I_1^2 \qquad K_5 = I_2$

$$\begin{aligned}3456K_6 = &- 5632I_4^3 + 18432I_9 - 1152I_3I_4^2 - 2592I_3^2I_4 - 1944I_3^3 + 55296I_2I_8 + 55296I_2^2I_7 + 21312I_2^2I_4^2 + 12960I_2^2I_3I_4\\ &+ 14580I_2^2I_3^2 + 18432I_2^3I_6 - 36936I_2^4I_4 - 36450I_2^4I_3 + 38151I_2^6 - 55296I_1I_8 - 110592I_1I_2I_7 - 40320I_1I_2I_4^2\\ &- 15552I_1I_2I_3I_4 - 17496I_1I_2I_3^2 - 55296I_1I_2^2I_6 + 121824I_1I_2^3I_4 + 87480I_1I_2^3I_3 - 156006I_1I_2^5 + 55296I_1^2I_7 + 20160I_1^2I_4^2\\ &+ 7776I_1^2I_3I_4 + 8748I_1^2I_3^2 + 55296I_1^2I_2I_6 - 167184I_1^2I_2^2I_4 - 96228I_1^2I_2^2I_3 + 302535I_1^2I_2^4 - 18432I_1^3I_6 + 106272I_1^3I_2I_4\\ &+ 52488I_1^3I_2I_3 - 339228I_1^3I_2^3 - 26568I_1^4I_4 - 13122I_1^4I_3 + 228177I_1^4I_2^2 - 86022I_1^5I_2 + 14337I_1^6\end{aligned}$$

$12L_1 = -4I_5 - 8I_2I_4 + 9I_2^3 + 6I_1I_3 - 18I_1I_2^2 + 9I_1^2I_2 - 2I_1^3$

$$\begin{aligned}288L_2 = &- 128I_4I_5 + 1536I_8 - 288I_3I_5 + 3072I_2I_7 - 192I_2I_4^2 - 288I_2I_3I_4 + 324I_2I_3^2 + 1536I_2^2I_6 + 720I_2^2I_5 + 1008I_2^3I_4 - 972I_2^3I_3\\ &+ 405I_2^5 - 3072I_1I_7 - 64I_1I_4^2 - 96I_1I_3I_4 + 108I_1I_3^2 - 3072I_1I_2I_6 - 864I_1I_2I_5 - 720I_1I_2^2I_4 + 1188I_1I_2^2I_3 - 1701I_1I_2^4\\ &+ 1536I_1^2I_6 + 432I_1^2I_5 - 144I_1^2I_2I_4 - 972I_1^2I_2I_3 + 3726I_1^2I_2^3 + 368I_1^3I_4 + 180I_1^3I_3 - 4014I_1^3I_2^2 + 2241I_1^4I_2 - 513I_1^5\end{aligned}$$

$$\begin{aligned}18L_3 = &- 96I_7 + 16I_4^2 + 36I_3I_4 - 96I_2I_6 - 36I_2I_5 - 162I_2^2I_4 + 81I_2^4 + 96I_1I_6 + 36I_1I_5 + 180I_1I_2I_4 + 54I_1I_2I_3 - 243I_1I_2^3 - 54I_1^2I_4\\ &- 54I_1^2I_3 + 243I_1^2I_2^2 - 99I_1^3I_2 + 18I_1^4\end{aligned}$$

$I_1 = K_5 + K_1 \qquad I_2 = K_5 \qquad I_3 = 2K_4 - 2K_2 + K_5^2 + K_1^2 \qquad 8I_4 = -12K_2 + 9K_1^2 \qquad I_5 = -3L_1 + 3K_5K_4 + K_5^3 + 3K_1K_4 - 3K_1K_2 + K_1^3$

$32I_6 = 6K_3 - 108K_1K_2 + 27K_1^3 \qquad 32I_7 = -6L_3 - 36K_2K_4 + 48K_2^2 - 36K_1L_1 + 6K_1K_3 + 27K_1^2K_4 - 144K_1^2K_2 + 27K_1^4$

$$\begin{aligned}32I_8 = &- 36K_4L_1 + 6L_2 + 48K_2L_1 - 12K_1L_3 + 27K_1K_4^2 - 144K_1K_2K_4 + 144K_1K_2^2 - 72K_1^2L_1 + 6K_1^2K_3 + 54K_1^3K_4\\ &- 180K_1^3K_2 + 27K_1^5\end{aligned}$$

$$\begin{aligned}32I_9 = &- 108K_2K_4^2 + 6K_6 + 27K_4^3 + 144K_2^2K_4 - 96K_2^3 + 18K_1L_2 - 108K_1K_4L_1 + 144K_1K_2L_1 - 18K_1^2L_3 + 81K_1^2K_4^2\\ &- 324K_1^2K_2K_4 + 288K_1^2K_2^2 - 108K_1^3L_1 + 6K_1^3K_3 + 81K_1^4K_4 - 216K_1^4K_2 + 27K_1^6\end{aligned}$$

Table 38: Polynomial relations between invariants of Tab. 4 or Tab. 11 and those proposed by Smith (1962) of group $\mathcal{T}_h$. $[\boldsymbol{a}_1] = (1,0,0)^\top$, $[\boldsymbol{a}_2] = (0,1,0)^\top$ and $[\boldsymbol{a}_3] = (0,0,1)^\top$.

$K_1 = I_1 \qquad 6K_2 = -I_3 + 2I_1^2 \qquad 54K_3 = -6I_7 - I_1I_3 + 2I_1^3 \qquad 6K_4 = -I_3 + 3I_2 - I_1^2$

$108K_5 = -36I_{10} - 18I_9 + 6I_2I_3 + 9I_2^2 + 24I_1I_8 + 24I_1I_7 - 14I_1^2I_3 - 6I_1^2I_2 + I_1^4 \qquad 54K_6 = -9I_8 - 6I_7 + 9I_4 + 8I_1I_3 - 9I_1I_2 + 2I_1^3$

$9L_1 = 3I_8 + 3I_7 - 4I_1I_3 + 3I_1I_2 - I_1^3$

$$\begin{aligned}324L_2 = &- 108I_{12} - 18I_3I_8 - 12I_3I_7 + 18I_2I_8 + 18I_2I_7 + 108I_1I_{10} + 18I_1I_9 + 16I_1I_3^2 - 60I_1I_2I_3 + 9I_1I_2^2 + 18I_1^2I_8 - 30I_1^2I_7\\ &+ 8I_1^3I_3 - 6I_1^3I_2 + I_1^5\end{aligned}$$

$108L_3 = 36I_{10} + 3I_3^2 - 15I_2I_3 + 12I_1I_8 - 12I_1I_7 - 5I_1^2I_3 + 6I_1^2I_2 - 2I_1^4 \qquad 3L_4 = 3I_6 + I_5 \qquad 3L_5 = -I_5$

$648L_6 = -216I_6I_8 + 216I_{14} + 9I_6I_7 - 75I_5I_8 - 24I_5I_7 + 39I_3I_{11} - 432I_1I_{13} + 141I_1I_3I_6 + 32I_1I_3I_5 + 288I_1^2I_{11} - 64I_1^3I_5$

$3L_7 = -I_{11} + I_1I_6 + I_1I_5 \qquad 18L_8 = 6I_{13} - I_3I_6 - 3I_2I_6 - I_2I_5 - 8I_1I_{11} + I_1^2I_6 + 3I_1^2I_5$

$I_1 = K_1 \qquad I_2 = 2K_4 - 2K_2 + K_1^2 \qquad I_3 = -6K_2 + 2K_1^2 \qquad I_4 = 3L_1 + 6K_6 + 3K_3 - 3K_1K_2 + K_1^3 \qquad I_5 = -3L_5 \qquad I_6 = L_5 + L_4$

$I_7 = -9K_3 + K_1K_2 \qquad I_8 = 3L_1 + 9K_3 - 2K_1K_4 - 7K_1K_2 + 2K_1^3$

$I_9 = -6L_3 - 6K_5 + 2K_4^2 + 2K_2K_4 + 2K_2^2 + 6K_1L_1 + 12K_1K_3 - 4K_1^2K_4 - 8K_1^2K_2 + 2K_1^4$

$I_{10} = 3L_3 - 5K_2K_4 + 2K_2^2 - K_1L_1 - 6K_1K_3 + 2K_1^2K_4 \qquad I_{11} = -3L_7 - 2K_1L_5 + K_1L_4$

$I_{12} = -3L_2 + K_4L_1 + 2K_2L_1 + 3K_2K_3 + 2K_1L_3 - K_1K_5 - 2K_1K_2K_4 - 3K_1K_2^2 - K_1^2K_3 + K_1^3K_2$

$I_{13} = 3L_8 + K_4L_4 - K_2L_5 - 2K_2L_4 - 4K_1L_7 - K_1^2L_5 + 2K_1^2L_4$

$$\begin{aligned}15I_{14} = &- 22K_1K_4L_5 + 45L_6 + 33L_1L_5 + 45L_1L_4 + 45K_3L_5 + 36K_3L_4 + 21K_2L_7 + 90K_1L_8 - 45K_1K_2L_5 - 79K_1K_2L_4\\ &- 67K_1^2L_7 + 45K_1^3L_4\end{aligned}$$

Table 39: Polynomial degrees of the proposed fundamental invariants in Tabs. 10 and 11 as well as the fundamental invariants K_α and L_β proposed by Smith (1962) for all considered groups. The invariants K_α and L_β of Smith (1962) are also listed in D.

Point group	Degree 1	Degree 2	Degree 3	Degree 4	Degree 5	Degree 6
$\mathcal{C}_i$	$\{I_1, I_2, I_3, I_4, I_5, I_6\}$ $\{K_1, K_2, K_3, K_4, K_5, K_6\}$	-	-	-	-	-
$\mathcal{C}_{1h}, \mathcal{C}_{2h}$	$\{I_1, I_2, I_3, I_4\}$ $\{K_1, K_2, K_3, K_4\}$	$\{I_5, I_6, I_7\}$ $\{K_5, K_6, L_1\}$	-	-	-	-
$\mathcal{C}_{2v}, \mathcal{D}_{2h}$	$\{I_1, I_2, I_3\}$ $\{K_1, K_2, K_3\}$	$\{I_4, I_5, I_6\}$ $\{K_4, K_5, K_6\}$	$\{I_7\}$ $\{L_1\}$	-	-	-
$\mathcal{C}_{2i}, \mathcal{C}_{4h}$	$\{I_1, I_2\}$ $\{K_1, K_3\}$	$\{I_3, I_4, I_5, I_6\}$ $\{K_2, K_4, K_6, L_3\}$	$\{I_7, I_8, I_9, I_{10}\}$ $\{L_1, L_2, L_4, L_5\}$	$\{I_{11}, I_{12}\}$ $\{K_5, L_6\}$	-	-
$\mathcal{C}_{4v}, \mathcal{D}_{2d}, \mathcal{D}_{4h}$	$\{I_1, I_2\}$ $\{K_1, K_3\}$	$\{I_3, I_4, I_5\}$ $\{K_2, K_4, K_6\}$	$\{I_6, I_7\}$ $\{L_1, L_2\}$	$\{I_8\}$ $\{K_5\}$	-	-
$\mathcal{C}_{3i}$	$\{I_1, I_2\}$ $\{K_1, K_4\}$	$\{I_3, I_4, I_5, I_6\}$ $\{K_2, K_5, L_1, L_4\}$	$\{I_7, I_8, I_9, I_{10}, I_{11}, I_{12}, I_{13}, I_{14}\}$ $\{K_3, K_6, L_2, L_3, L_5, L_6, L_7, L_8\}$	-	-	-
$\mathcal{C}_{3v}, \mathcal{D}_{3d}$	$\{I_1, I_2\}$ $\{K_1, K_4\}$	$\{I_3, I_4, I_5\}$ $\{K_2, K_5, L_1\}$	$\{I_6, I_7, I_8, I_9\}$ $\{K_3, K_6, L_2, L_3\}$	-	-	-
$\mathcal{C}_{3h}, \mathcal{C}_{6h}$	$\{I_1, I_2\}$ $\{K_1, K_5\}$	$\{I_3, I_4\}$ $\{K_2, K_4\}$	$\{I_5, I_6, I_7, I_8\}$ $\{K_3, L_1, L_4, L_5\}$	$\{I_9, I_{10}\}$ $\{L_3, L_7\}$	$\{I_{11}, I_{12}\}$ $\{L_2, L_8\}$	$\{I_{13}, I_{14}\}$ $\{K_6, L_6\}$
$\mathcal{C}_{6v}, \mathcal{D}_{3h}, \mathcal{D}_{6h}$	$\{I_1, I_2\}$ $\{K_1, K_5\}$	$\{I_3, I_4\}$ $\{K_2, K_4\}$	$\{I_5, I_6\}$ $\{K_3, L_1\}$	$\{I_7\}$ $\{L_3\}$	$\{I_8\}$ $\{L_2\}$	$\{I_9\}$ $\{K_6\}$
$\mathcal{T}_h$	$\{I_1\}$ $\{K_1\}$	$\{I_2, I_3\}$ $\{K_2, K_4\}$	$\{I_4, I_5, I_6, I_7, I_8\}$ $\{K_3, K_6, L_1, L_4, L_5\}$	$\{I_9, I_{10}, I_{11}\}$ $\{K_5, L_3, L_7\}$	$\{I_{12}, I_{13}\}$ $\{L_2, L_8\}$	$\{I_{14}\}$ $\{L_6\}$
$\mathcal{T}_d, \mathcal{O}_h$	$\{I_1\}$ $\{K_1\}$	$\{I_2, I_3\}$ $\{K_2, K_4\}$	$\{I_4, I_5, I_6\}$ $\{K_3, K_6, L_1\}$	$\{I_7, I_8\}$ $\{K_5, L_3\}$	$\{I_9\}$ $\{L_2\}$	-

F Syzygies between proposed fundamental invariants

Some syzygies, relevant to this work, between the fundamental invariants of Tabs. 10 and 11 in higher polynomial degrees are presented below. These allow for a distinction between primary and secondary invariants.

Table 40: Syzygies between the fundamental invariants of Tabs. 10 and 11.

Group	Syzygy
C_{1h}	$I_1^2 I_3^2 = -I_5 I_7 + 2I_7^2 + 2I_6^2 - 2I_4^2 I_7 + I_4^2 I_5 - 4I_3 I_4 I_6 - 2I_3^2 I_7 + I_3^2 I_5 + 2I_3^2 I_4^2 - 4I_2 I_4 I_6 + 2I_2 I_3 I_7 + 2I_2 I_3 I_4^2 - 2I_2 I_3^3 + 2I_2^2 I_7 - 2I_2^2 I_3^2 - 2I_1 I_3 I_7 + 2I_1 I_3 I_4^2 + 2I_1 I_3^3 - 2I_1 I_2 I_7 + 2I_1 I_2 I_4^2 + 2I_1 I_2 I_3^2 + I_1^2 I_7 - I_1^2 I_4^2$
C_{2h}	$4I_1^4 = -4I_5^2 + 16I_7^2 + 16I_6^2 + 4I_4^2 I_5 - I_4^4 + 4I_3^2 I_5 - 2I_3^2 I_4^2 - I_3^4 + 32I_2 I_4 I_7 + 32I_2 I_3 I_6 + 12I_2^2 I_5 + 10I_2^2 I_4^2 + 10I_2^2 I_3^2 - 9I_2^4 + 16I_1 I_2 I_5 - 8I_1 I_2 I_4^2 - 8I_1 I_2 I_3^2 - 24I_1 I_2^3 + 8I_1^2 I_5 - 4I_1^2 I_4^2 - 4I_1^2 I_3^2 - 28I_1^2 I_2^2 - 16I_1^3 I_2$
$C_\infty, C_{\infty h}$	$2I_1^6 = -36I_2 I_4 I_5 + 36I_6^2 + 4I_5^2 + 36I_4^3 + 90I_3 I_4^2 + 72I_3^2 I_4 + 18I_3^3 - 24I_2 I_3 I_5 - 18I_2^2 I_3 I_4 - 9I_2^2 I_3^2 + 12I_2^3 I_5 - 24I_1 I_4 I_5 - 24I_1 I_3 I_5 - 72I_1 I_2 I_4^2 - 108I_1 I_2 I_3 I_4 - 36I_1 I_2 I_3^2 + 48I_1 I_2^2 I_5 - 54I_1^2 I_4^2 - 72I_1^2 I_3 I_4 - 18I_1^2 I_3^2 + 48I_1^2 I_2 I_5 + 54I_1^2 I_2^2 I_4 + 18I_1^2 I_2^2 I_3 + 16I_1^3 I_5 + 72I_1^3 I_2 I_4 + 24I_1^3 I_2 I_3 - 12I_1^3 I_2^3 + 24I_1^4 I_4 + 6I_1^4 I_3 - 21I_1^4 I_2^2 - 12I_1^5 I_2$

References

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