research papers

Automatic calculation of symmetry-adapted tensors in magnetic and non-magnetic materials: a new tool of the Bilbao Crystallographic Server

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Two new programs, *MTENSOR* and *TENSOR*, hosted on the open-access website known as the Bilbao Crystallographic Server, are presented. The programs provide automatically the symmetry-adapted form of tensor properties for any magnetic or non-magnetic point group or space group. The tensor is chosen from a list of 144 known tensor properties gathered from the scientific literature or, alternatively, the user can also build a tensor that possesses an arbitrary intrinsic symmetry. Four different tensor types are considered: equilibrium, transport, optical and nonlinear optical susceptibility tensors. For magnetically ordered structures, special attention is devoted to a detailed discussion of the transformation rules of the tensors under the time-reversal operation 1'. It is emphasized that for non-equilibrium properties it is the Onsager theorem, and not the constitutive relationships, that indicates how these tensors transform under 1'. In this way it is not necessary to restrict the validity of Neumann's principle. New Jahn symbols describing the intrinsic symmetry of the tensors are introduced for several transport and optical properties. In the case of some nonlinear optical susceptibilities of practical interest, an intuitive method is proposed based on simple diagrams, which allows easy deduction of the action of 1' on the susceptibilities. This topic has not received sufficient attention in the literature and, in fact, it is usual to find published results where the symmetry restrictions for such tensors are incomplete.

1. Introduction

The analysis of the restrictions that space–time symmetry produces in the tensors describing the properties of magnetically ordered crystals has been a research subject for more than 50 years (Birss, 1963, 1964; Cracknell, 1973; Eremenko *et al.*, 1992; Grimmer, 1993, 1994, 2017; Kleiner, 1966; Kopsky, 2015; Landau & Lifshitz, 1960; Litvin & Litvin, 1991; Shtrikman & Thomas, 1965; Sirotin & Shaskolskaya, 1982). The topic is interesting because the tensor form determines whether a particular physical phenomenon can take place in the crystal, and also regulates the anisotropy of the different material properties.

For tensors that describe equilibrium properties, the restrictions derived from the application of Neumann's principle to the constitutive equation that defines the tensor property lead directly to the final form of the considered tensor. The relevant point group is one of the 122 magnetic point groups first derived by Shubnikov & Belov (1964). In the reduction process it must be taken into account that the operations that contain time reversal 1' change the sign of the tensor if it is of magnetic type, *i.e.* if there are an odd

Λ_{ij}	j					
i	1	2	3	4	5	6
1	0	0	0	0	Λ_{15}	$-2\Lambda_{22}$
2	$-\Lambda_{22}$	Λ_{22}	0	Λ_{15}	0	0
3	Λ_{31}	Λ_{31}	Λ_{33}	0	0	0

number of magnetic vectors in the constitutive relation. Otherwise the tensor remains invariant under $1'$.

The procedure to obtain the restrictions imposed by symmetry in the case of non-equilibrium properties is more complicated. As early as 1963, Birss (1963) realized that the application of the operations which contain $1'$ in the reduction process from the constitutive relations leads to absurd results, even for dia- and paramagnetic crystals. For example, it would appear that the existence of electrical conductivity is forbidden in all 32 grey point groups: under time reversal, the electric current density vector **J** changes its sign, whereas the electric field **E** remains invariant. Thus, the conductivity tensor relating both vectors should vanish in all time-symmetric crystals. In view of this paradox, Birss proposed to restrict the validity of Neumann's principle to operations that do not contain time reversal for dynamic (*i.e.* entropy-producing) properties. However, after a 20-year dispute it was established that the behaviour of the tensors under time reversal must be determined not by the constitutive equations but by the Onsager relationships (Butzal & Birss, 1982; Eremenko *et al.*, 1992; Grimmer, 1994; Shtrikman & Thomas, 1965). In other words, it is the Onsager theorem that tells us the way these tensors transform under $1'$ and also allows a consistent application of Neumann's principle to these kinds of tensors. Non-equilibrium tensors include not only the tensors for transport properties (*e.g.* electrical or thermal conductivities, diffusion phenomena or thermoelectric effects) but also the optical tensors. In this respect, it is important to note that the response of a crystal to an electromagnetic field cannot be described as an equilibrium phenomenon unless the frequencies involved are low enough (Eremenko *et al.*, 1992).

Although in the literature the shapes of the symmetry-adapted tensors in both non-magnetic and magnetic crystals have been discussed many times (Eremenko *et al.*, 1992; Grimmer, 1993, 1994; Kleiner, 1966; Newnham, 2005; Nye, 1985; Shtrikman & Thomas, 1965; Tinder, 2008), we have found it interesting to make an exhaustive compilation of tensor properties and offer a simple automatic procedure to obtain the tensor forms in any of the crystallographic magnetic point groups. With this aim we have implemented a program, called *MTENSOR*, within the Bilbao Crystallographic Server (http://www.cryst.ehu.es/cryst/mtensor). On the server there is also a simplified version of the program, named *TENSOR*, which is appropriate for non-magnetic crystals (see http://www.cryst.ehu.es/cryst/tensor). *TENSOR* provides information on the symmetry-adapted tensors for non-magnetic materials, as a function of their ordinary point group, without the need to consider magnetic symmetry. This information can also be retrieved from *MTENSOR* if instead the magnetic grey point group (or space group) corresponding to the relevant ordinary (non-magnetic) group is introduced as input.

MTENSOR provides the symmetry-adapted form of tensor properties for any magnetic point (or space) group. On the one hand, a point group must be selected. On the other hand, a tensor must be defined by the user, or selected from the lists of known equilibrium, transport and optical tensors gathered from the scientific literature. If a standard magnetic point or space group is defined and a known tensor is selected from the lists, the program will return the required tensor from an internal database. Otherwise, the tensor is calculated live.

MTENSOR is linked from a database of magnetic structures, called MAGNDATA (Gallego *et al.*, 2016), which is also hosted on the Bilbao Crystallographic Server (http://www.cryst.ehu.es/magndata).

In this paper we give a detailed description of the working principles of *MTENSOR*. We will begin with tensors associated with equilibrium properties. We will then illustrate the procedure followed for tensors of transport properties. Finally, we will deal with optical tensors, with a special discussion of the form that the Onsager relationships take for some nonlinear optical susceptibilities of practical interest. We propose an intuitive method based on simple diagrams, which allows the determination of the action of the $1'$ operation on any optical susceptibility. This topic has not been considered sufficiently in the literature. In fact, even in recent publications it is usual to find partial reductions of such tensors following just the old incomplete Birss prescription.

2. Equilibrium properties

In the case of tensors describing static properties, their transformation laws under the action of the operations of a magnetic point group are well known (Birss, 1964). The kind of transformation depends on the number of axial vectors that are involved in the constitutive relation, as well as on the number of magnetic vectors. These numbers determine the polar or axial character of the tensor (even or odd number of axial vectors, respectively) and the non-magnetic or magnetic character (even or odd number of magnetic vectors, respectively). For example, for the magnetoelectric tensor of rank 2, a_{ij}, which relates an applied electric field E_j (polar non-magnetic vector) to an induced magnetization M_i (axial magnetic vector) through the constitutive relation $M_i = a_{ij}E_j$, we have the symmetry relations

$$a_{ij} = |R|R_{im}R_{jn}a_{mn}, \tag{1}$$

for the proper or improper operations R of the point group that do not include time reversal, and

$$a_{ij} = -|R|R_{im}R_{jn}a_{mn}, \tag{2}$$

for the operations $R' = R1'$ that include the time-reversal operation $1'$. In (1) and (2) R_{ij} are the elements of the 3×3 matrices that represent the point-group operations R in the orthonormal basis in which the constitutive relation is also expressed, and $|R|$ is the determinant of the matrix.

We will use Jahn's notation (Jahn, 1949) to designate the kind of tensor according to its transformation properties. The magnetoelectric tensor has rank 2 (V^2), and it is axial (*e*) and magnetic (*a*), so it is labelled aeV^2. Using this notation, additional symmetries like symmetry or antisymmetry of pairs of indices are easily incorporated through square brackets or curly brackets. For example, the elastic tensor C_{ijkl} is of type $[[V^2][V^2]]$. This means a polar non-magnetic tensor of rank 4, symmetric in indices i, j, also symmetric in indices k, l, and

where, additionally, the pair i, j is interchangeable by k, l. Similarly, a tensor V_{ijk} of type $a\{V^2\}V$ would be a magnetic tensor of rank 3 antisymmetric in indices i, j. In *MTENSOR* we present a list of 60 equilibrium properties with 24 different Jahn symbols. For a given point group, tensor properties that are forbidden by symmetry are listed on a grey background. Among rank 1 tensors we have included the four basic ferroic effects: electric polarization vector P_i of type V, magnetization vector M_i of type aeV, polar toroidal moment T_i of type aV and axial toroidal moment A_i of type eV. The rank of the considered tensors ranges between 1 and 8. The main page and an example of the output of *MTENSOR* are given in Fig. 1.

When a tensor of third rank or higher is symmetric under the permutation of two indices i and j, the tensor is given in abbreviated notation by making the substitution $ij \rightarrow u$ ($i, j = 1, 2, 3$; $u = 1, \ldots, 6$). The usual Voigt-like correspondence $11 \rightarrow 1, 22 \rightarrow 2, 33 \rightarrow 3, 23 \rightarrow 4, 13 \rightarrow 5, 12 \rightarrow 6$ is adopted (Nye, 1985). However, although it is customary to introduce factors of 1/2 (or even 1/4 in some cases) into the relationships between some of the coefficients expressed in abbreviated and full-tensor notations, we will not follow this convention here. The correspondence between coefficients is always taken with unity factors to unify the wide variety of cases presented by the different tensors. For example, our elastic compliance coefficients in abbreviated notation verify $S_{11} = S_{1111}$, $S_{16} = S_{1112}$ or $S_{45} = S_{2313}$. Similarly, the piezoelectric coefficients fulfil $d_{11} = d_{111}$ or $d_{36} = d_{312}$, exactly like the stiffness coefficients C_{ij} and C_{ijkl}. This contrasts with the convention used in the book by Nye (1985). Therefore, care should be taken when writing the constitutive relationships or expressions for the crystal energy using the abbreviated notation. These equations can only be written in compact form using the full-tensor notation.

In cases of higher symmetry, where more than two indices can be interchanged, the abbreviated notation is used for the first two indices on the left and, if possible, the next two indices on the right are treated in the same way. For example, if the Jahn symbol is $[V^3]$ the correspondence is $T_{uk} = T_{ijk}$, $u = 1, \ldots, 6$ and $i, j, k = 1, 2, 3$. If the symbol is $[V^4]$ double reduction is possible and the correspondence is $T_{uv} = T_{ijkl}$, $u, v = 1, \ldots, 6$ and $i, j, k, l = 1, 2, 3$.

3. Transport properties

In the section on transport properties, *MTENSOR* deals with more than 20 different phenomena related to diffusion, thermal conduction, electrical conduction and combined effects: electrodiffusion, thermodiffusion and thermoelectric effects. Also, we incorporate variations in these properties upon application of external magnetic fields, especially the Hall, Nernst and Ettinghausen effects. In total we find six different Jahn symbols for the tensors, whose ranks are between 2 and 4. As was mentioned in Section 1, the reduction of tensor transport properties involves the Onsager reciprocity theorem to obtain the transformation law of the tensors upon the time-reversal operation $1'$. To explain how Onsager relationships enable us to find out the effect of $1'$ on these tensors, we will give below an example considering the case of thermoelectric effects (Grimmer, 1993, 2017).

Let us take a crystal where a temperature gradient ∇T and an electric current with density current $\mathbf{J}$ have been established. Then a thermal current with heat-flux density $\mathbf{q}$ and an electric field $\mathbf{E}$ are produced. In the absence of diffusion phenomena these quantities are related as

$$E_i = \rho_{ij}(\mathbf{S}, \mathbf{H})J_j + \beta_{ij}(\mathbf{S}, \mathbf{H})(\nabla T)_j,$$
$$q_i = T\pi_{ij}(\mathbf{S}, \mathbf{H})J_j - k_{ij}(\mathbf{S}, \mathbf{H})(\nabla T)_j, \tag{3}$$

where we have explicitly written the dependence of the tensor properties on the spin configuration $\mathbf{S}$ of the crystal and the value of a possible external magnetic field $\mathbf{H}$. In equation (3) ρ_{ij} is the electrical resistivity tensor, k_{ij} the thermal conduc-

MTENSOR: Tensor calculation for Magnetic Point Groups

For the symmetry-adapted form of non-magnetic crystal tensors see TENSOR

Tensor calculation for Magnetic Point Groups

MTENSOR provides the symmetry-adapted form of tensor properties for any magnetic point (or space) group. On the one hand, a point or space group must be selected. On the other hand, a tensor must be defined by the user or selected from the lists of known equilibrium, optical, nonlinear optical susceptibility and transport tensors, gathered from scientific literature. If a magnetic point or space group is defined and a known tensor is selected from the lists the program will obtain the required tensor from an internal database; otherwise, the tensor is calculated live. Live calculation of tensors may take too much time and even exceed the time limit, giving an empty result, if high-rank tensors, and/or a lot of symmetry elements are introduced.

Further information can be found here

Please, enter a magnetic point group or a magnetic space group:

Magnetic Point or Space Group number: choose it

Please, choose a tensor by one of these ways:

● **Choose a tensor from the lists**

☐ Show symmetry-adapted tensors for all the magnetic point groups in standard setting
(this overrides previous choices)

EQUILIBRIUM TENSORS

OPTICAL TENSORS

NONLINEAR OPTICAL SUSCEPTIBILITY TENSORS

TRANSPORT TENSORS

○ **Build your own tensor**

- Introduce Jahn's symbol without superscripts. Examples: (1) [[V2][V2]], (2) a{V2}*, (3) (V2[V2])*

Get results

(a)

Symmetry-adapted form of the Piezomagnetic tensor Λ_{ijk} (direct effect) for the magnetic point group 32' (#18.3.67)

Information about the selected tensor

- 3rd rank Piezomagnetic tensor Λ_{ijk} (direct effect)
- Axial tensor which inverts under time-reversal symmetry operation
- Defining equation: $M_i = \Lambda_{ijk}\sigma_{jk}$
- Relates Stress tensor σ_{ij} with Magnetization $\mathbf{M}$
- Intrinsic symmetry symbol: aeV[V²]
- Symmetrized indexes due to intrinsic symmetry:
  - $\Lambda_{ijk} = \Lambda_{ikj}$
- Abbreviated notation: $\Lambda_{ijk} \rightarrow \Lambda_{ij}$
  - jk → j if j=k, jk → 9-(j+k) if j≠k

Table of tensor components

Λ_{ij}		j					
		1	*2*	*3*	*4*	*5*	*6*
i	*1*	0	0	0	0	Λ_{15}	$-2\Lambda_{22}$
	2	$-\Lambda_{22}$	Λ_{22}	0	Λ_{15}	0	0
	3	Λ_{31}	Λ_{31}	Λ_{33}	0	0	0

Number of independent coefficients: 4

Note: semitransparent tensor components are identical or opposite to bold symbols due to the intrinsic symmetry of the tensor

(b)

Figure 1
(*a*) The main page of *MTENSOR* and (*b*) a typical output provided by the program. An example is given of the symmetry-adapted form of the piezomagnetic tensor for the magnetic point group 32′, together with some relevant information on the chosen property.

tivity, and β_{ij} and $T\pi_{ij}$ the tensors for the Seebeck and Peltier effects, respectively. All these tensors can be grouped as a 6×6 matrix in the form

$$L(\mathbf{S}, \mathbf{H}) = \begin{pmatrix} \rho & \beta \\ \pi & -k \end{pmatrix}, \qquad (4)$$

which is the matrix of the kinetic coefficients of the thermoelectric effects. Onsager's theorem can be written as a symmetry relation of the kinetic coefficients (Grimmer, 1993, 2017):

$$L_{ij}(\mathbf{S}, \mathbf{H}) = L_{ji}(-\mathbf{S}, -\mathbf{H}). \qquad (5)$$

As can be seen, this expression can be understood as a transformation law of the kinetic coefficients by time reversal, since spins and magnetic fields are reversed by that operation. Therefore, for the diagonal tensors of matrix $L_{ij}(\mathbf{S}, \mathbf{H})$ we deduce the following relations:

$$1'\rho_{ij}(\mathbf{S}, \mathbf{H}) = \rho_{ij}(-\mathbf{S}, -\mathbf{H}) = \rho_{ji}(\mathbf{S}, \mathbf{H}), \qquad (6)$$

$$1'k_{ij}(\mathbf{S}, \mathbf{H}) = k_{ij}(-\mathbf{S}, -\mathbf{H}) = k_{ji}(\mathbf{S}, \mathbf{H}). \qquad (7)$$

Similarly, for the nondiagonal tensors we have

$$1'\beta_{ij}(\mathbf{S}, \mathbf{H}) = \beta_{ij}(-\mathbf{S}, -\mathbf{H}) = \pi_{ji}(\mathbf{S}, \mathbf{H}), \qquad (8)$$

$$1'\pi_{ij}(\mathbf{S}, \mathbf{H}) = \pi_{ij}(-\mathbf{S}, -\mathbf{H}) = \beta_{ji}(\mathbf{S}, \mathbf{H}). \qquad (9)$$

Therefore, the action of the primed elements $R' = R1'$ of the crystal point group on the diagonal tensors is

$$\rho_{ij} = R_{im}R_{jn}\rho_{nm}, \qquad (10)$$

and an identical equation for k_{ij}. On the other hand, for elements R which do not contain time reversal we have the usual relationship:

$$\rho_{ij} = R_{im}R_{jn}\rho_{mn}, \qquad (11)$$

and the same for k_{ij}. These transformation laws (10) and (11) define a non-standard Jahn symbol which we will denote as $[V^2]*$ (emphasizing the fact that $1'\rho_{ij} = \rho_{ji}$). In the case of a non-magnetic crystal, equation (6) implies $\rho_{ij} = \rho_{ji}$. In other words, for grey groups (groups containing the $1'$ operation) the Jahn symbol $[V^2]*$ gives the same restrictions as $[V^2]$.

In general, if ρ_{ij} is written as the sum of a symmetric and an antisymmetric part $\rho_{ij} = \rho_{ij}^S + \rho_{ij}^A$, it is easily deduced that ρ^S is a $[V^2]$ tensor and ρ^A an $a\{V^2\}$ tensor. According to Grimmer (2017), to treat ρ^S and ρ^A as separate tensors leads to simpler and stronger results. In this way it can be shown that ρ^S accounts for the ordinary ohmic resistivity and ρ^A is responsible for the so-called spontaneous Hall effect, which does not produce energy dissipation. In *MTENSOR* we do not explicitly separate ρ^S and ρ^A. However, both tensors can easily be deduced from ρ by taking its symmetric and antisymmetric parts.

The nondiagonal tensors of matrix $L_{ij}(\mathbf{S}, \mathbf{H})$ have different transformation properties. From (8) and (9) it can be seen that elements R' do not place any restriction on the tensor shape, but relate elements of tensors that describe different properties. Thus, we have the transformations

$$\pi_{ij} = R_{im}R_{jn}\beta_{nm} \qquad (12)$$

and

$$\beta_{ij} = R_{im}R_{jn}\pi_{nm}, \qquad (13)$$

which connect the Seebeck and Peltier coefficients.

The only reduction for the individual tensors π and β then comes from the non-primed operations in the usual way,

$$\pi_{ij} = R_{im}R_{jn}\pi_{mn}, \qquad (14)$$

and a similar equation for β. These kinds of tensor will be denoted by the symbol $(V^2)*$ (here we have $1'\pi_{ij} = \beta_{ji}$). For grey groups, $\beta_{ij} = \pi_{ji}$.

If we consider jointly the effects of electrical conduction, thermal conduction and diffusion, the kinetic coefficients can be written as a 9×9 matrix L_{ij}, which verifies new Onsager relationships similar to equation (5). In this case there are three diagonal properties of type $[V^2]*$ (the third one is the diffusion tensor) and six nondiagonal tensors related to each other in pairs. The latter are tensors of type $(V^2)*$.

The application of external magnetic fields leads to the definition of new effects that can be described by means of tensors of ranks higher than 2. For tensors of type $[V^2]*$, like ρ_{ij}, a magnetic field gives rise to a dependence of the resistivity that can be written approximately as a Taylor series,

$$\rho_{ij}(\mathbf{H}) = \rho_{ij}(0) + R_{ijk}H_k + T_{ijkl}H_kH_l + \dots. \qquad (15)$$

$\rho_{ij}(0)$ is the zero-order term, R_{ijk} is the tensor for the Hall effect ($E_i = R_{ijk}J_jH_k$) and T_{ijkl} is the tensor for magnetic resistance ($E_i = T_{ijkl}J_jH_kH_l$).

Taking into account that $\mathbf{H}$ is an axial magnetic vector, the following transformation properties can be deduced.

For the subgroup of non-primed operations R,

$$R_{ijk} = |R|R_{im}R_{jn}R_{ks}R_{mns} \qquad (16)$$

and

$$T_{ijkl} = R_{im}R_{jn}R_{ks}R_{lp}T_{mnsp}, \qquad (17)$$

and for primed operations R',

$$R_{ijk} = -|R|R_{im}R_{jn}R_{ks}R_{nms} \qquad (18)$$

and

$$T_{ijkl} = R_{im}R_{jn}R_{ks}R_{lp}T_{nmsp}. \qquad (19)$$

These transformation laws mean that $1'R_{ijk} = -R_{jik}$ and $1'T_{ijkl} = T_{jikl}$. Accordingly, the intrinsic symmetry of the R and T tensors will be denoted by the new Jahn symbols $e\{V^2\}*V$ and $[V^2]*[V^2]$, respectively. It can be checked that for grey groups the Jahn symbols $\{\}*$ and $[]*$ give the same restrictions as $\{\}$ and $[]$, respectively

Similar to the case of ρ_{ij}, we can separate the Hall tensor into an antisymmetric part, $R_{ijk}^A = -R_{jik}^A$ of type $e\{V^2\}V$ (ordinary Hall effect), and a symmetric part, $R_{ijk}^S = R_{jik}^S$, responsible for the (anomalous) linear magnetoresistance, which is of $ae[V^2]V$ type. In the same way, the tensor T is separable into a symmetric part, $T_{ijkl}^S = T_{jikl}^S$, which describes the (ordinary) quadratic magnetoresistance (type $[V^2][V^2]$), and an antisymmetric part, $T_{ijkl}^A = -T_{jikl}^A$ ($a\{V^2\}[V^2]$), respon-

Table 1
Intrinsic symmetry of some tensors describing thermoelectric effects.

The symmetric and antisymmetric parts of the tensors account for different properties. The symmetric and antisymmetric tensors are not explicitly included in *MTENSOR* but can easily be obtained from the full original tensor. $\rho_{ij}(\mathbf{H}) = \rho_{ij}(0) + R_{ijk}H_k + T_{ijkl}H_kH_l$, $k_{ij}(\mathbf{H}) = k_{ij}(0) + Q_{ijk}H_k + S_{ijkl}H_kH_l$.

Tensor	Intrinsic symmetry	Property	Symmetric part	Antisymmetric part
ρ_{ij}	$[V^2]^*$	Electrical resistivity	$[V^2]$, ordinary resistivity $(\rho_{ij} + \rho_{ji})/2$	$a\{V^2\}$, spontaneous Hall effect $(\rho_{ij} - \rho_{ji})/2$
k_{ij}	$[V^2]^*$	Thermal conductivity	$[V^2]$, ordinary thermal conductivity $(k_{ij} + k_{ji})/2$	$a\{V^2\}$, spontaneous Righi–Leduc effect $(k_{ij} - k_{ji})/2$
R_{ijk}	$e\{V^2\}^*V$	Hall effect	$ae[V^2]V$, linear magnetoresistence $(R_{ijk} + R_{jik})/2$	$a\{V^2\}V$, ordinary Hall effect $(R_{ijk} - R_{jik})/2$
T_{ijkl}	$[V^2]^*[V^2]$	Magnetoresistence	$[V^2][V^2]$, quadratic magnetoresistence $(T_{ijkl} + T_{jikl})/2$	$a\{V^2\}[V^2]$, quadratic anomalous Hall effect $(T_{ijkl} - T_{jikl})/2$
Q_{ijk}	$e\{V^2\}^*V$	Righi–Leduc effect	$ae[V^2]V$, linear magneto-heat conductivity $(Q_{ijk} + Q_{jik})/2$	$e\{V^2\}V$, ordinary Righi–Leduc effect $(Q_{ijk} - Q_{jik})/2$
S_{ijkl}	$[V^2]^*[V^2]$	Magneto-heat conductivity	$[V^2][V^2]$, quadratic magneto-heat conductivity $(S_{ijkl} + S_{jikl})/2$	$a\{V^2\}[V^2]$, quadratic anomalous Righi–Leduc effect $(S_{ijkl} - S_{jikl})/2$

Table 2
Some of the tensors without internal symmetry that describe thermoelectric effects.

New tensors with enhanced symmetry can be constructed from them by appropriate linear combinations. From a pair of tensors a new pair is built. One tensor in each pair is invariant and the other changes sign under $1'$. These new tensors account for properties with different physical interpretations. They are not explicitly included in *MTENSOR* but can be obtained from the information available in the program. $\pi_{ij}(\mathbf{H}) = \pi_{ij}(0) + M_{ijk}H_k$, $\beta_{ij}(\mathbf{H}) = \beta_{ij}(0) + N_{ijk}H_k$.

Tensor	Intrinsic symmetry	Property	Non-magnetic part (invariant under $1'$)	Magnetic part (changes sign under $1'$)
π_{ij}	$(V^2)^*$	Peltier effect	V^2, ordinary Peltier effect $(\pi_{ij} + \beta_{ji})/2$	aV^2, spontaneous Ettinghausen effect $(\pi_{ij} - \beta_{ji})/2$
β_{ij}	$(V^2)^*$	Seebeck effect	$[V^2]$, ordinary Seebeck effect $(\beta_{ij} + \pi_{ji})/2$	$a\{V^2\}$, spontaneous Righi–Leduc effect $(\beta_{ij} - \pi_{ji})/2$
M_{ijk}	$(eV^3)^*$	Ettinghausen effect	eV^3, ordinary Ettinghausen effect $(M_{ijk} - N_{jik})/2$	aeV^3, linear magneto-Peltier effect $(M_{ijk} + N_{jik})/2$
N_{ijk}	$(eV^3)^*$	Nernst effect	eV^3, ordinary Nernst effect $(N_{ijk} - M_{jik})/2$	aeV^3, linear magneto-Seebeck effect $(N_{ijk} + M_{jik})/2$

sible for the (anomalous) quadratic Hall effect. Again, these separations are not explicitly carried out in *MTENSOR* but can be obtained from the full R_{ijk} and T_{ij} tensors.

For nondiagonal tensors, the application of a magnetic field leads to a series expansion similar to equation (15). Taking the Peltier tensor as an example, we have

$$\pi_{ij}(\mathbf{H}) = \pi_{ij}(0) + M_{ijk}H_k + \ldots, \qquad (20)$$

where M_{ijk} is the tensor for the so-called Ettinghausen effect. That tensor is of type $(eV^3)^*$, which means a transformation rule

$$M_{ijk} = |R|R_{im}R_{jn}R_{kl}M_{mnl}, \qquad (21)$$

for non-primed operations R, and an Onsager-like relationship for primed operations R',

$$M_{ijk} = -|R|R_{im}R_{jn}R_{kl}N_{nml}, \qquad (22)$$

which in this case is not useful for further tensor reduction. In equation (22) N_{ijk} is the tensor for the Nernst effect, which involves the Seebeck instead of the Peltier coefficients in an expression like (20) $[\beta_{ij}(\mathbf{H}) = \beta_{ij}(0) + N_{ijk}H_k + \ldots]$. As can be seen, the Onsager relationships (22) connect the Ettinghausen and Nernst coefficients.

A combination of the M and N tensors can be devised that leads to new tensors which are either invariant or change sign under $1'$. These tensors describe a series of ordinary (non-magnetic) and anomalous (magnetic) effects, respectively, and have been compiled by Grimmer (2017).

In Tables 1 and 2 we have gathered some important thermoelectric effects showing the intrinsic symmetry of the relevant tensors.

4. Optical properties

Optical properties are based on the behaviour of the dielectric permittivity tensor at optical frequencies and its variation due to external stimuli, such as electric fields, magnetic fields, stress, strain *etc.*

As has been described in the section on static properties (Section 2), the dielectric tensor is of type $[V^2]$ for fields of sufficiently slow variation. However, this is no longer the case for optical frequencies because the material response cannot be considered as an equilibrium phenomenon. It can be shown that at these frequencies the dielectric tensor must satisfy the Onsager relationships (Eremenko *et al.*, 1992),

$$\varepsilon_{ij}(\mathbf{k}, \mathbf{S}, \mathbf{H}) = \varepsilon_{ji}(-\mathbf{k}, -\mathbf{S}, -\mathbf{H}), \qquad (23)$$

where $\mathbf{k}$ is the light wavevector, $\mathbf{S}$ specifies the spin configuration in magnetic materials and $\mathbf{H}$ is an external magnetic field. Upon time reversal, all $\mathbf{k}$, $\mathbf{S}$ and $\mathbf{H}$ change direction, so equation (23) means that the transformation of the optical dielectric tensor under the $1'$ operation is

$$1'\varepsilon_{ij}(\mathbf{k}, \mathbf{S}, \mathbf{H}) = \varepsilon_{ji}(\mathbf{k}, \mathbf{S}, \mathbf{H}). \qquad (24)$$

In other words, at optical frequencies ε_{ij} becomes a $[V^2]^*$ tensor.

Table 3
Spontaneous optical properties allowing space dispersion up to second order.

Tensor	Intrinsic symmetry	Optical property	Real or imaginary character in non-dissipative media
$(\varepsilon_{ij}^0)^S$	$[V^2]$	Index ellipsoid	Real
$(\varepsilon_{ij}^0)^A$	$a\{V^2\}$	Spontaneous Faraday effect	Imaginary
γ_{ijl}^A	$\{V^2\}V$	Natural optical activity†	Real
γ_{ijl}^S	$a[V^2]V$	Spontaneous gyrotropic birefringence‡	Imaginary
$\gamma_{ijkl}^{(2)S}$	$[V^2][V^2]$	Birefringence in cubic crystals	Real
$\gamma_{ijkl}^{(2)A}$	$a\{V^2\}[V^2]$	Non-mutual optical activity‡	Imaginary

† In experimental work, gyrotropy is sometimes treated using a gyrotropic axial tensor $g_{lk} = (k_0/2)\varepsilon_{ijk}\gamma_{ijl}^A$, which is expressed in terms of the completely antisymmetric Levi–Civita axial tensor ε_{ijk} and the modulus of the light wavevector in a vacuum k_0. The magnitude of the gyration G is given through the symmetric part of g_{lk} as $G = g_{lk}k_lk_k/k_0^2$. The non-symmetric part of g_{lk} is not observable.   ‡ Not observed yet.

The variation in ε_{ij} due to space dispersion (dependence on **k**), application of electric or magnetic fields and other external influences can be expanded in a Taylor series thus:

$$\varepsilon_{ij} = \varepsilon_{ij}^0 + i\gamma_{ijl}k_l + \gamma_{ijlm}^{(2)}k_lk_m + \ldots + r_{ijl}E_l + R_{ijlk}E_lE_k + \ldots$$
$$\ldots + iz_{ijl}H_l + C_{ijlk}H_lH_k + \ldots . \qquad (25)$$

Every tensor in (25) is responsible for an optical effect, with its own intrinsic symmetry. In this way we deduce the following symmetries: the zero-order ε_{ij}^0 is a $[V^2]^*$ tensor, which describes the index ellipsoid of the crystal, γ_{ijl} is a tensor of type $\{V^2\}^*V$ since **k** changes sign upon application of $1'$, $\gamma_{ijlm}^{(2)}$ is of type $[V^2]^*[V^2]$, r_{ijl} has an intrinsic symmetry $[V^2]^*V$ and R_{ijlk} is $[V^2]^*[V^2]$. Finally, z_{ijl} is of type $e\{V^2\}^*V$ and C_{ijlk} is $[V^2]^*[V^2]$.

In their turn, all these tensors have symmetric and antisymmetric parts with respect to transpositions of indices i and j. We first examine the spontaneous effects. A list of them is given in Table 2. If, in addition, the medium is non-dissipative, ε_{ij} must be Hermitian ($\varepsilon_{ij} = \varepsilon_{ji}^*$) (Landau & Lifshitz, 1960). This condition implies that all elements of the symmetric and antisymmetric tensors are either real or purely imaginary. The last column of Table 3 accounts for this point. In the case of dissipative media all tensors are complex.

Regarding the disturbances of the dielectric tensor caused by external electric or magnetic fields, r_{ijk} is responsible for the electro-optic Pockels effect, R_{ijkl} is the electro-optic Kerr tensor, z_{ijk} accounts for the Faraday effect and C_{ijkl} is the tensor corresponding to the Cotton–Moutton effect. In *MTENSOR* only the main (non-magnetic) effects associated with these tensors are considered, except for the Faraday and Cotton–Mouton effects. In the first case we include the possibility of a symmetric part of z_{ijk} in the indices i and j, $q_{ijk} = iz_{ijk}^S$ with $q_{ijk} = q_{jik}$, which corresponds to the so-called magneto-optic Kerr effect. In the second case we consider a possible antisymmetric part of C_{ijkl} in the indices i and j, $B_{ijkl} = iC_{ijkl}^A$, with $B_{ijkl} = -B_{jikl}$. This phenomenon is named the quadratic magneto-optic Kerr effect. The two magneto-optic

Table 4
Tensors describing alterations of ε_{ij} due to electric and magnetic fields.

Tensor	Intrinsic symmetry	Optical property	Real or imaginary character in non-dissipative media
r_{ijk}^S	$[V^2]V$	Pockels effect	Real
R_{ijkl}^S	$[V^2][V^2]$	Kerr effect	Real
z_{ijk}^A	$e\{V^2\}V$	Faraday effect	Real
$q_{ijk} = iz_{ijk}^S$	$ae[V^2]V$	Magneto-optic Kerr effect	Real
C_{ijkl}^S	$[V^2][V^2]$	Cotton–Mouton effect	Real
$B_{ijkl} = iC_{ijkl}^A$	$a\{V^2\}[V^2]$	Quadratic magneto-optic Kerr effect	Real

Kerr effects are only observable in magnetically ordered materials. All these tensors are real in non-dissipative media (see Table 4).

Apart from these effects, *MTENSOR* also takes account of further alterations in the permittivity due to other external perturbations such as stress, strain or the effect of combined fields. Tensor shapes are analysed up to rank 6.

5. Nonlinear optical susceptibilities

Nonlinear optical phenomena have recently been revealed as a powerful tool for the investigation of magnetic symmetries, structures and interactions in magnetically ordered crystals (Dähn *et al.*, 1996; Fiebig *et al.*, 1994, 1996, 2005; Kirilyuk, 2002; Pavlov *et al.*, 2002; Pisarev, 1996, 2013; Pisarev *et al.*, 2010; Yokota *et al.*, 2012). Among the great variety of nonlinear optical effects we will focus mainly on electric dipole effects, which are usually associated with the most prominent phenomena. At the end of this section we will briefly consider some examples involving magnetic dipole effects.

We will adopt the usual notation $\chi_{i_n i_{n-1} \ldots i_1}(\omega_n; \omega_{n-1}, \ldots, \omega_1)$ ($\omega_n \geq 0$) to designate an $(n-1)$-nonlinear susceptibility where input electric field waves of frequencies $\omega_{n-1}, \ldots, \omega_1$ produce an electric polarization at a frequency $\omega_n = \omega_{n-1} + \ldots + \omega_1$. This polarization then acts as source term in the wave equation, giving rise to an electric field that also oscillates at a frequency ω_n. In short, frequencies on the right-hand side of the semicolon are those of the input waves. They can be positive or negative (a negative frequency is understood as an output wave with positive frequency). The frequency on the left-hand side of the semicolon represents the frequency of the output wave (always positive or null).

As in previous cases, in order to obtain the restrictions that the symmetry of a magnetic group produces on these tensors, the crucial point is to find out the way they behave under time reversal, *i.e.* we need the appropriate Onsager relationships. This problem has received scant attention in the literature. In the work of Naguleswaran & Stedman (1996, 1998), some relations were derived starting from the quantum mechanical expressions for the susceptibilities. Here, we will follow a simpler procedure well adapted to our needs.

The procedure is based on the assignment of simple diagrams to the different optical properties. The action of time

reversal on a given susceptibility is obtained by just inverting the event sequence in the diagram describing that process. The new diagram corresponds to a new process, which is readily identified. As far as we know, this method has never been used before for these purposes. The validity of the results of the method will be checked by comparison with well known Onsager relationships in particular cases.

We start with a simple linear process with one input wave and one output wave, both of frequency ω. Instead of the permittivity ε_{ij} we will use the equivalent susceptibility tensor $\chi_{ij}(\omega;\omega)$. In this notation, the process described by $\chi_{ij}(\omega;\omega)$ is the production of an output wave of frequency ω polarized along i from an input electric wave of frequency ω polarized along j. The process is shown schematically in Fig. 2(a). Now let us consider the time-reversed process. Under time reversal the input and output are interchanged, so we have the scheme in Fig. 2(b). This new process is driven by $\chi_{ji}(\omega;\omega)$, so we arrive at the conclusion

$$1'\chi_{ij}(\omega;\omega) = \chi_{ji}(\omega;\omega), \tag{26}$$

which is the well known Onsager relation for the dielectric permittivity (Eremenko et al., 1992).

We now extend the use of these diagrams to higher-order processes. Let us examine a general second-order process driven by $\chi_{ijk}(\omega_3;\omega_2,\omega_1)$ and shown schematically in Fig. 3(a). The time-reversed process is shown in Fig. 3(b) and, as can be seen, the tensor component associated with it is either $\chi_{jik}(\omega_2;\omega_3,-\omega_1)$ or, equivalently, $\chi_{kij}(\omega_1;\omega_3,-\omega_2)$. Therefore we should have

$$1'\chi_{ijk}(\omega_3;\omega_2,\omega_1) = \chi_{jik}(\omega_2;\omega_3,-\omega_1) = \chi_{kij}(\omega_1;\omega_3,-\omega_2). \tag{27}$$

This is the Onsager relation for the process. In contrast with the linear case, equation (27) only provides us with a relationship between elements of different tensor properties, and thus it is not useful to reduce the tensor. We have here a situation similar to the one found previously for the non-
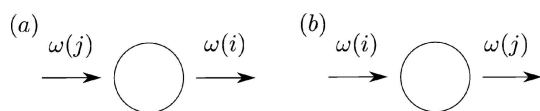

Figure 2
(a) The linear process in which one input wave of frequency ω polarized along the j axis gives rise to an output wave of frequency ω oscillating along i. Under time reversal the process (b) is obtained, where the roles of i and j are interchanged.
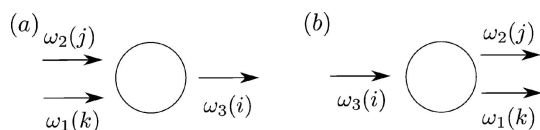

Figure 3
(a) A general second-order process in which two waves of frequencies ω_1 and ω_2 combine to generate a wave of frequency $\omega_3 = \omega_1 + \omega_2$. (b) The time-reversed process. ω_3 is an input frequency and the output can be chosen between ω_2 ($\omega_2 = \omega_3 - \omega_1$) or ω_1 ($\omega_1 = \omega_3 - \omega_2$).

Table 5
Intrinsic symmetry of tensors describing some second- and third-order nonlinear optical effects in dissipative crystals.

Optical property	Tensor	Intrinsic symmetry
General second-order process	$\chi_{ijk}(\omega_3;\omega_2,\omega_1)$	$(V^3)*$
Second-harmonic generation	$\chi_{ijk}(2\omega;\omega,\omega)$	$(V[V^2])*$
Pockels effect	$\chi_{ijk}(\omega;\omega,0)$	$[V^2]*V$
Optical rectification	$\chi_{ijk}(0;\omega,-\omega)$	$V[V^2]*$
General third-order process	$\chi_{ijkl}(\omega_4;\omega_3,\omega_2,\omega_1)$	$(V^4)*$
Four-wave mixing	$\chi_{ijkl}(\omega_1;-\omega_2,\omega_1,\omega_2)$	$[V^2V^2]*$
Degenerate four-wave mixing	$\chi_{ijkl}(\omega;-\omega,\omega,\omega)$	$[[V^2][V^2]]*$

diagonal blocks in equation (4) when dealing with some transport properties. This is not strange because the direct and reversed processes correspond to different physical phenomena. For example, if $\omega_1 > 0$ and $\omega_2 > 0$, the direct and time-reversed processes are a sum-frequency and a difference-frequency generation, respectively. Therefore, in general, we can only use the non-primed elements of the magnetic point group to reduce the tensor. The intrinsic symmetry of the susceptibility will be $(V^3)*$.

Only in some special cases, when the direct and reversed processes are of the same nature, is equation (27) useful for further tensor reduction. This happens when one of the frequencies of the input waves is the same as that of one of the output waves (the case $\omega = 0$ does not count). In the second-order case there are only two relevant situations, which are shown schematically in Fig. 4.

The first case [Fig. 4(a)] is controlled by $\chi_{ijk}(\omega;\omega,0)$. In fact, it is nothing but the electro-optic Pockels effect, with a susceptibility proportional to the Pockels tensor $\chi_{ijk}(\omega;\omega,0) \propto r_{ijk}$. The reversed process is driven by $\chi_{jik}(\omega;\omega,0)$ [or alternatively by $\chi_{kij}(0;\omega,-\omega)$]. This means that

$$1'\chi_{ijk}(\omega;\omega,0) = \chi_{jik}(\omega;\omega,0), \tag{28}$$

or

$$1'\chi_{ijk}(\omega;\omega,0) = \chi_{kij}(0;\omega,-\omega). \tag{29}$$

Equation (28) gives the already known relationship (Eremenko et al., 1992) for the Pockels tensor $1'r_{ijk} = r_{jik}$ with intrinsic symmetry $[V^2]*V$. Equations (29) and (28) express a relationship between the tensors for the Pockels effect and for the so-called optical rectification phenomenon, consisting of the generation of a DC electric field upon illumination with an intense light beam.
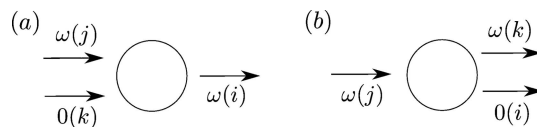

Figure 4
(a) A second-order process in which a wave of frequency ω polarized along the j axis is transformed into a wave of the same frequency polarized along i due to the interaction with a static electric field applied along the k axis. (b) The optical rectification phenomenon. A DC field along the i axis is generated by the interaction of two waves of frequency ω oscillating along j and k.

Table 6
Intrinsic symmetry of some nonlinear optical tensors for non-dissipative crystals and for media showing no dispersion.

Optical property	Tensor	Real part	Imaginary part	Kleinman symmetry
General second-order process	$\chi_{ijk}(\omega_3; \omega_2, \omega_1)$	V^3	aV^3	Real $[V^3]$
Second-harmonic generation	$\chi_{ijk}(2\omega; \omega, \omega)$	$V[V^2]$	$aV[V^2]$	Real $[V^3]$
Optical rectification	$\chi_{ijk}(0; \omega, -\omega)$	$V[V^2]$	$aV\{V^2\}$	Real $[V^3]$
General third-order process	$\chi_{ijkl}(\omega_4; \omega_3, \omega_2, \omega_1)$	V^4	aV^4	Real $[V^4]$
Electric field-induced second-harmonic generation	$\chi_{ijkl}(2\omega; 0, \omega, \omega)$	$V^2[V^2]$	$aV^2[V^2]$	Real $[V^4]$
Third-harmonic generation	$\chi_{ijkl}(3\omega; \omega, \omega, \omega)$	$V[V^3]$	$aV[V^3]$	Real $[V^4]$
General second-order process by magnetic dipole	$\chi_{ijk}^{m}(\omega_3; \omega_2, \omega_1)$	aeV^3	eV^3	Imaginary $e[V^3]$
Second-harmonic generation by magnetic dipole	$\chi_{ijk}^{m}(2\omega; \omega, \omega)$	$aeV[V^2]$	$eV[V^2]$	Imaginary $e[V^3]$

In Fig. 4(b) we show just the optical rectification process $\chi_{ijk}(0;\omega,-\omega)$. The time-reversed process is driven by $\chi_{ikj}(0;\omega,-\omega)$, so

$$1'\chi_{ijk}(0; \omega, -\omega) = \chi_{ikj}(0; \omega, -\omega). \qquad (30)$$

Thus, the Jahn symbol for this tensor must be $V[V^2]^*$.

For third-order processes, the most general case where we can associate input and output waves in conjugate pairs is shown schematically in Fig. 5. It corresponds to the four-wave mixing process. From the figure we easily deduce

$$1'\chi_{ijkl}(\omega_1; -\omega_2, \omega_1, \omega_2) = \chi_{klij}(\omega_1; -\omega_2, \omega_1, \omega_2). \qquad (31)$$

Thus, the intrinsic symmetry of this property is $[V^2V^2]^*$.

A special case of the above effect is the so-called degenerate four-wave mixing process, when all frequencies are the same. Obviously we have

$$1'\chi_{ijkl}(\omega; -\omega, \omega, \omega) = \chi_{klij}(\omega; -\omega, \omega, \omega), \qquad (32)$$

but here we have still more reduction because kl and ij can also be interchanged. Then the tensor is $[[V^2][V^2]]^*$.

Table 5 gives the intrinsic symmetry of some important tensors for electric dipole second- and third-order effects.

It is interesting to point out that further reduction can be achieved in the case of non-dissipative media. We will show the reason for this by analysing the case for the second-order susceptibility. It can be shown that the absence of dissipation implies a second-order electric dipole response (Klyshko, 2011; Popov *et al.*, 1995),

$$\chi_{ijk}(\omega_3; \omega_2, \omega_1) = \left[\chi_{jik}(\omega_2; \omega_3, -\omega_1)\right]^* = \left[\chi_{kji}(\omega_1; -\omega_2, \omega_3)\right]^*. \qquad (33)$$

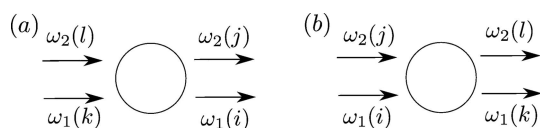Therefore equations (27) and (33) give

Figure 5
(a) A third-order process in which two waves of frequencies ω_2 polarized along the j and l axes, and another wave of frequency ω_1 polarized along k, combine to produce a wave of frequency ω_1 oscillating along the i axis. (b) The time-reversed process can be interpreted as the direct process with an interchange of indices i and j by k and l, respectively.

$$1'\chi_{ijk}(\omega_3; \omega_2, \omega_1) = \left[\chi_{ijk}(\omega_3; \omega_2, \omega_1)\right]^*, \qquad (34)$$

i.e. we regain a relationship between elements of the same tensor property. Equation (34), first deduced by Pershan (1963), then permits the use of primed operations of the magnetic point group to reduce the susceptibility tensor further.

Interestingly, although equation (34) implies that dia- and paramagnetic transparent crystals have real susceptibilities (since for them $1'$ is always a symmetry operation), this is not necessarily the case in magnetically ordered materials, even if they are lossless. In fact, for the magnetic point group 1 it can be shown that all tensor elements are complex. The real and imaginary parts can then be interpreted as separate contributions to the susceptibility coming from the crystal structure and the spin configuration, respectively.

Table 6 is a catalogue of nonlinear optical tensors showing their intrinsic symmetry for lossless media. The last column gives the intrinsic symmetry of the tensor property, assuming additionally that the medium has no dispersion (also known as Kleinman symmetry; Kleinman, 1962).

To find the Kleinman condition, we consider non-dissipative media and neglect the frequency dependence of the susceptibility. In the second-order case, the general symmetry conditions for the susceptibility $\chi_{ijk}(\omega_3;\omega_2, \omega_1) = \chi_{ikj}(\omega_3;\omega_1, \omega_2)$, together with equation (33) specific for non-dissipative media, give

$$\chi_{ijk}(\omega_3; \omega_2, \omega_1) = \chi_{ikj}(\omega_3; \omega_1, \omega_2)$$
$$= \left[\chi_{jik}(\omega_2; \omega_3, -\omega_1)\right]^*$$
$$= \left[\chi_{jki}(\omega_2; -\omega_1, \omega_3)\right]^*$$
$$= \left[\chi_{kji}(\omega_1; -\omega_2, \omega_3)\right]^*$$
$$= \left[\chi_{kij}(\omega_1; \omega_3, -\omega_2)\right]^*. \qquad (35)$$

If, in addition, we omit the frequency arguments because of the lack of dispersion, we have

$$\chi_{ijk} = \chi_{ikj} = \left[\chi_{jik}\right]^* = \left[\chi_{jki}\right]^* = \left[\chi_{kji}\right]^* = \left[\chi_{kij}\right]^*. \qquad (36)$$

Now, if we take the real part of the χ tensor, which is of type V^3, we see from equation (36) that every pair of indices can be permuted, so V^3 transforms into $[V^3]$. On the other hand, the imaginary part of χ must be symmetric in the last two indices (since $\chi_{ijk} = \chi_{ikj}$) and antisymmetric in the first two (since $\chi_{ijk} = $

$[\chi_{jik}]^*$). This implies $\text{Im}\,\chi = 0$. Similar reasoning can be applied to the third-order susceptibility.

To end this section we will give a brief account of some second-order susceptibility tensors that involve magnetic dipole effects. The transformation laws associated with these susceptibilities can easily be deduced from those of their electric dipole counterparts by just noting that a magnetic axial vector replaces an electric vector in their constitutive equations. Then the behaviour under time reversal can be obtained by just adding a minus sign. For example, equation (27) becomes

$$1'\chi_{ijk}^{\mathrm{m}}(\omega_3; \omega_2, \omega_1) = -\chi_{jik}^{\mathrm{m}}(\omega_2; \omega_3, -\omega_1) = -\chi_{kij}^{\mathrm{m}}(\omega_1; \omega_3, -\omega_2),$$
(37)

where the superscript m makes reference to a magnetic dipole susceptibility. In general, if there are k magnetic vectors involved in the constitutive relation for the susceptibility, we should include a $(-1)^k$ factor in the transformation law.

It is easy to understand that, as a rule, direct and time-reversed susceptibilities that involve magnetic dipole effects are of different natures, similar to the electric dipole case. Again, the case of non-dissipative media permits further reduction. As shown by Pershan (1963), the equivalent of equation (34) is now

$$1'\chi_{ijk}^{\mathrm{m}}(\omega_3; \omega_2, \omega_1) = -\left[\chi_{ijk}^{\mathrm{m}}(\omega_3; \omega_2, \omega_1)\right]^*.$$
(38)

The last two rows of Table 6 give two examples of second-order magnetic dipole effects. Remarkably, both tensors are purely imaginary for media without dispersion or for non-magnetic crystals.

In *MTENSOR* a list of 31 nonlinear susceptibilities is presented. All the effects gathered in Tables 5 and 6 are included, analysing separately the cases of dissipative and non-dissipative materials, and also examining the possibility of having the Kleinman symmetry. Only second- and third-order effects are considered, with a total of 25 different Jahn symbols.

6. Concluding remarks

In this paper we have presented a new tool of the Bilbao Crystallographic Server. We have implemented two new programs, *MTENSOR* and *TENSOR*, which enable the user to obtain automatically the shapes of the symmetry-adapted tensors of magnetic and non-magnetic crystals. Four categories of tensor have been considered: equilibrium, transport, optical and nonlinear optical susceptibility tensors. For all of these we have discussed their behaviour under 1'. For the last kind of tensor we have also given an intuitive graphical method for the easy deduction of their transformation rules under time reversal.

More than 140 different properties are compiled, with tensor ranks between 1 and 8. Although many different intrinsic tensor symmetries are considered, the programs also offer the possibility of building any tensor *à la carte*. This is useful if the user is interested in a tensor whose symmetry is not found in the lists.

An interesting extension for both programs would be a tool that permitted the derivation of the symmetry-adapted form of the tensor properties for all the corresponding domain-related equivalent structures arising at a phase transition (Litvin, 2014). In *TENSOR*, this would require the specification of the space group of the structure, the parent space group and, optionally, the transformation relating the settings of both structures. In *MTENSOR* the non-magnetic to magnetic phase transitions seem to be the most interesting. In this case we would have to specify the space group of the parent phase together with the magnetic subgroup of the daughter phase. The construction of these tools is our plan for the near future.

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