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On physical property tensors invariant under line groups[1]

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The form of physical property tensors of a quasi-one-dimensional material such as a nanotube or a polymer can be determined from the point group of its symmetry group, one of an *infinite* number of line groups. Such forms are calculated using a method based on the use of trigonometric summations. With this method, it is shown that materials invariant under infinite subsets of line groups have physical property tensors of the same form. For line group types of a family of line groups characterized by an index n and a physical property tensor of rank m, the form of the tensor for all line group types indexed with $n > m$ is the same, leaving only a *finite* number of tensor forms to be determined.

1. Introduction

Non-magnetic and magnetic line groups (Hermann, 1928; Alexander, 1929; Damnjanović & Vujičić, 1982) describe the symmetry of quasi-one-dimensional materials, as polymers (Vainshtein, 1966) and nanotubes (Damnjanović & Milošević, 2010). The form of tensors representing physical properties of such materials is invariant under the point groups, referred to here as *line point groups* (also known as *axial point groups*), of these line groups. The 31 families of line point group types (Damnjanović & Vujičić, 1981), which categorize the infinite number of line groups, are listed in Table 1. These line point groups are subdivided into three subclasses: (i) groups $\mathbf{G}$ which do not contain the time inversion operation $1'$, neither by itself nor coupled with another element; (ii) groups $\mathbf{G1'}$ which are direct products of a group $\mathbf{G}$ of the first subclass and the group $\mathbf{1'} = \{1,1'\}$; and (iii) groups $\mathbf{G}(\mathbf{H}) = \mathbf{H} + (\mathbf{G} - \mathbf{H})1'$ where $\mathbf{H}$ is a subgroup of index two of a group $\mathbf{G}$ of the first subclass, of elements not coupled with time inversion, and the remaining elements of $\mathbf{G}$, *i.e.* the elements $\mathbf{G} - \mathbf{H}$, are coupled with the time inversion.

Let V represent a three-dimensional polar vector and $V^m = V \times V \times \ldots \times V$ the mth ranked product of V (Jahn, 1949). An mth rank physical property tensor V^m in three-dimensional space has 3^m components. Each component of V can be indexed, when using a Cartesian coordinate system, by the symbols x, y and z of the coordinate system. Each component of V^m can then be indexed by an ordered product of m x, y and z's. We shall refer to these products as *m-products*. Let e and a denote zero-rank tensors that change sign under spatial inversion $\bar{1}$ and time inversion $1'$, respectively. Combining these tensors with tensors V^m we have the four types of tensors of mth ranked physical property tensors V^m, eV^m, aV^m and aeV^m considered in this paper.

In §2, new methods are set out to determine the form of property tensors invariant under individual finite and infinite (limiting) line point groups. In §3, using these methods and a corollary of Hermann's theorem (Hermann, 1934), we derive a general bypass theorem which enables one to bypass having to determine the form of individual property tensors under all line point groups by showing that the form of the tensors is the same under infinite subsets of line point groups. This theorem is applied in §4 along with the methods of §2 to tabulate the form of all rank-two magnetic and non-magnetic physical property tensors, including those with internal symmetry, invariant under all line point groups.

2. Physical property tensors invariant under line point groups

Given an mth rank physical property tensor and a group $\mathbf{G}$ whose elements are denoted by G_q, $q = 1, 2, \ldots, |\mathbf{G}|$, where $|\mathbf{G}|$ denotes the order of the group $\mathbf{G}$, one determines conditions on the form of the tensor invariant under $\mathbf{G}$ by applying each element G_q of $\mathbf{G}$ to each of the 3^m components of the tensor. Applying an element G_q to a component of the tensor gives rise to a linear combination of components. Equating the original component with this combination gives a condition which the components must satisfy if the tensor is to be invariant under $\mathbf{G}$. That is, for each of the 3^m components of the mth ranked tensor and $|\mathbf{G}|$ elements G_q of $\mathbf{G}$, we have $3^m|\mathbf{G}|$ conditions on the components that the tensor must satisfy to be invariant under $\mathbf{G}$. These conditions are

$$\text{component}_s = G_q\,(\text{component}_s) \qquad (1)$$

for $s = 1, 2, \ldots, 3^m$ and $q = 1, 2, \ldots, |\mathbf{G}|$.

From Table 1 we see that each line point group is a group $\mathbf{C}_n$ or contains a subgroup $\mathbf{C}_n$ of index two, four or eight.

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Table 1
Families of line point group types.

$\mathbf{C}_n$ denotes the family of line group types with n = 1, 2, 3, … of groups generated by a rotation of $2\pi/n$ about an axis which we take as the major axis. σ_v is a vertical mirror plane, a plane containing the z axis, σ_h a horizontal mirror plane, perpendicular to the major axis, U a twofold rotation perpendicular to the major axis, and U_d a twofold rotation perpendicular to the major axis and halfway between neighboring vertical mirror planes. To the right of the group symbol is the coset decomposition of the line point group with respect to its subgroup $\mathbf{C}_n$.

Groups **G**	
$\mathbf{C}_n$	
$\mathbf{C}_{nv}$	$= \mathbf{C}_n + \sigma_v \mathbf{C}_n$
$\mathbf{S}_{2n}$	$= \mathbf{C}_n + (\sigma_h C_{2n}) \mathbf{C}_n$
$\mathbf{C}_{nh}$	$= \mathbf{C}_n + \sigma_h \mathbf{C}_n$
$\mathbf{D}_n$	$= \mathbf{C}_n + U \mathbf{C}_n$
$\mathbf{D}_{nd}$	$= \mathbf{C}_{nv} + U_d \mathbf{C}_{nv} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + U_d\mathbf{C}_n + U_d\sigma_v \mathbf{C}_n$
$\mathbf{D}_{nh}$	$= \mathbf{C}_{nv} + \sigma_h \mathbf{C}_{nv} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + \sigma_h \mathbf{C}_n + \sigma_h \sigma_v \mathbf{C}_n$
Groups **G1′**	
$\mathbf{C}_n\mathbf{1}'$	$= \mathbf{C}_n + 1' \mathbf{C}_n$
$\mathbf{C}_{nv}\mathbf{1}'$	$= \mathbf{C}_{nv} + 1' \mathbf{C}_{nv} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + 1'(\mathbf{C}_n + \sigma_v \mathbf{C}_n)$
$\mathbf{S}_{2n}\mathbf{1}'$	$= \mathbf{S}_{2n} + 1' \mathbf{S}_{2n} = \mathbf{C}_n + (\sigma_h C_{2n}) \mathbf{C}_n + 1'(\mathbf{C}_n + (\sigma_h C_{2n}) \mathbf{C}_n)$
$\mathbf{C}_{nh}\mathbf{1}'$	$= \mathbf{C}_{nh} + 1' \mathbf{C}_{nh} = \mathbf{C}_n + \sigma_h \mathbf{C}_n + 1'(\mathbf{C}_n + \sigma_v \mathbf{C}_n)$
$\mathbf{D}_n\mathbf{1}'$	$= \mathbf{D}_n + 1' \mathbf{D}_n = \mathbf{C}_n + U \mathbf{C}_n + 1'(\mathbf{C}_n + U \mathbf{C}_n)$
$\mathbf{D}_{nd}\mathbf{1}'$	$= \mathbf{D}_{nd} + 1' \mathbf{D}_{nd} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + U_d\mathbf{C}_n + U_d\sigma_v \mathbf{C}_n + 1'(\mathbf{C}_n + \sigma_v \mathbf{C}_n + U_d\mathbf{C}_n + U_d\sigma_v \mathbf{C}_n)$
$\mathbf{D}_{nh}\mathbf{1}'$	$= \mathbf{D}_{nh} + 1' \mathbf{D}_{nh} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + \sigma_h \mathbf{C}_n + \sigma_h \sigma_v \mathbf{C}_n + 1'(\mathbf{C}_n + \sigma_v \mathbf{C}_n + \sigma_h \mathbf{C}_n + \sigma_h \sigma_v \mathbf{C}_n)$
Groups **G**(**H**)	
$\mathbf{C}_{2n}(\mathbf{C}_n)$	$= \mathbf{C}_n + C_{2n}' \mathbf{C}_n$
$\mathbf{S}_{2n}(\mathbf{C}_n)$	$= \mathbf{C}_n + (\sigma_h C_{2n})' \mathbf{C}_n$
$\mathbf{C}_{nh}(\mathbf{C}_n)$	$= \mathbf{C}_n + \sigma_h' \mathbf{C}_n$
$\mathbf{C}_{2nh}(\mathbf{S}_{2n})$	$= \mathbf{S}_{2n} + \sigma_h' \mathbf{S}_{2n} = \mathbf{C}_n + (\sigma_h C_{2n}) \mathbf{C}_n + \sigma_h'(\mathbf{C}_n + (\sigma_h C_{2n}) \mathbf{C}_n)$
$\mathbf{C}_{2nh}(\mathbf{C}_{nh})$	$= \mathbf{C}_{nh} + C_{2n}' \mathbf{C}_{nh} = \mathbf{C}_n + \sigma_h \mathbf{C}_n + C_{2n}'(\mathbf{C}_n + \sigma_h \mathbf{C}_n)$
$\mathbf{D}_n(\mathbf{C}_n)$	$= \mathbf{C}_n + U' \mathbf{C}_n$
$\mathbf{D}_{2n}(\mathbf{D}_n)$	$= \mathbf{D}_n = C_{2n}' \mathbf{D}_n = \mathbf{C}_n + U \mathbf{C}_n + C_{2n}'(\mathbf{C}_n + U \mathbf{C}_n)$
$\mathbf{C}_{nv}(\mathbf{C}_n)$	$= \mathbf{C}_n + \sigma_v' \mathbf{C}_n$
$\mathbf{C}_{2nv}(\mathbf{C}_{nv})$	$= \mathbf{C}_{nv} + C_{2n}' \mathbf{C}_{nv} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + C_{2n}'(\mathbf{C}_n + \sigma_v \mathbf{C}_n)$
$\mathbf{D}_{nd}(\mathbf{S}_{2n})$	$= \mathbf{S}_{2n} + U_d' \mathbf{S}_{2n} = \mathbf{C}_n + (\sigma_h C_{2n}) \mathbf{C}_n + U_d'(\mathbf{C}_n + (\sigma_h C_{2n}) \mathbf{C}_n)$
$\mathbf{D}_{nd}(\mathbf{D}_n)$	$= \mathbf{D}_n + \sigma_v' \mathbf{D}_n = \mathbf{C}_n + U_d\mathbf{C}_n + \sigma_v'(\mathbf{C}_n + U_d\mathbf{C}_n)$
$\mathbf{D}_{nd}(\mathbf{C}_{nv})$	$= \mathbf{C}_{nv} + U_d' \mathbf{C}_{nv} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + U_d'(\mathbf{C}_n + \sigma_v \mathbf{C}_n)$
$\mathbf{D}_{nh}(\mathbf{C}_{nh})$	$= \mathbf{C}_{nh} + \sigma_v' \mathbf{C}_{nh} = \mathbf{C}_n + \sigma_h \mathbf{C}_n + \sigma_v'(\mathbf{C}_n + \sigma_h \mathbf{C}_n)$
$\mathbf{D}_{nh}(\mathbf{D}_n)$	$= \mathbf{D}_n + \sigma_h' \mathbf{D}_n = \mathbf{C}_n + U \mathbf{C}_n + \sigma_h'(\mathbf{C}_n + U \mathbf{C}_n)$
$\mathbf{D}_{nh}(\mathbf{C}_{nv})$	$= \mathbf{C}_{nv} + \sigma_h' \mathbf{C}_{nv} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + \sigma_h'(\mathbf{C}_n + \sigma_v \mathbf{C}_n)$
$\mathbf{D}_{2nh}(\mathbf{D}_{nd})$	$= \mathbf{D}_{nd} + C_{2n}' \mathbf{D}_{nd} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + U_d\mathbf{C}_n + U_d\sigma_v \mathbf{C}_n + C_{2n}'(\mathbf{C}_n + \sigma_v \mathbf{C}_n + U_d \mathbf{C}_n + U_d\sigma_v \mathbf{C}_n)$
$\mathbf{D}_{2nh}(\mathbf{D}_{nh})$	$= \mathbf{D}_{nh} + C_{2n}' \mathbf{D}_{nh} = \mathbf{C}_n + \sigma_v \mathbf{C}_n + \sigma_h \mathbf{C}_n + \sigma_h \sigma_v \mathbf{C}_n + C_{2n}'(\mathbf{C}_n + \sigma_v \mathbf{C}_n + \sigma_h \mathbf{C}_n + \sigma_h \sigma_v \mathbf{C}_n)$

Consequently, the form of every physical property tensor invariant under any line point group is invariant under a group $\mathbf{C}_n$. Therefore, we shall begin by determining a method to find the form of tensors V^m invariant under line point groups $\mathbf{C}_n$. Subsequently, we shall use this method as a basis to determine the form of all tensors of rank m invariant under all line point groups.

In determining the form of tensors V^m invariant under line point groups $\mathbf{C}_n$, since the transformational properties of the components of V^m under elements of $\mathbf{C}_n$ are the same as the transformational properties m-products of x, y and z under elements of $\mathbf{C}_n$, equation (1) can be rewritten as

$$m\text{-product}_s = (C_n)_q\,(m\text{-product}_s), \tag{2}$$

$s = 1, 2, \ldots, 3^m$ and $q = 1, 2, \ldots, |\mathbf{C}_n|$.

Groups $\mathbf{C}_n$, $n = 1, 2, 3, \ldots\ \infty$, constitute an infinite series of point groups associated with line groups. We shall consider only cases $n > 1$ since for $n = 1$, $\mathbf{C}_1 = \{1\}$ where '1' is the identity element, and the invariance of V^m under $\mathbf{C}_1$ gives the general form of the physical property tensor. Each group $\mathbf{C}_n$, $n = 1, 2, 3, \ldots\ \infty$, is generated by a single element C_n, a rotation of $2\pi/n$ about what we choose as the z axis, and the elements of $\mathbf{C}_n$, for a specific n, can be denoted by $(C_n)^j$, $j = 1, 2, \ldots, n$, where n is the order $|\mathbf{C}_n|$ of the group $\mathbf{C}_n$. As this cyclic group is generated by the single element C_n, a tensor whose components satisfy the 3^m conditions of equation (2) for the element C_n, *i.e.*

$$m\text{-product}_s = C_n\,(m\text{-product}_s) \tag{3}$$

for $s = 1, 2, \ldots, 3^m$, automatically satisfies (see Appendix *A* in the supporting information[2]) the $3^m\,(n-1)$ conditions

$$m\text{-product}_s = (C_n)^j\,(m\text{-product}_s) \tag{4}$$

for $s = 1, 2, \ldots, 3^m$ and $j = 2, 3, \ldots, n$.

Combining for each m-product$_s$ the sum of equation (3) and equation (4) for $j = 2, 3, \ldots, n$, assuming that n is finite, we have that a physical property tensor V^m invariant under $\mathbf{C}_n$ satisfies the 3^m conditions

$$n(m\text{-product}_s) = \sum_{j=1}^{n} (C_n)^j (m\text{-product}_s) \tag{5}$$

for $s = 1, 2, \ldots, 3^m$. In Appendix *A*, it is also shown that the m-products which satisfy equation (5) also satisfy equations (3) and (4). Consequently, in determining the form of a tensor V^m invariant under a group $\mathbf{C}_n$ one can replace the $n3^m$ conditions of equations (3) and (4) with the 3^m conditions of equation (5).

We shall use equation (5) to generate conditions on the form of physical property tensors V^m invariant under the group $\mathbf{C}_n$. The right-hand side of equation (5) is evaluated by considering the action of the element $(C_n)^j$ on each index of the m-product. This action is that

$$\text{each } x \text{ is replaced with } x\cos\left(\frac{2\pi}{n}\right)j - y\sin\left(\frac{2\pi}{n}\right)j, \tag{6a}$$

$$\text{each } y \text{ is replaced with } x\ \sin\left(\frac{2\pi}{n}\right)j + y\cos\left(\frac{2\pi}{n}\right)j, \tag{6b}$$

and each z is left unchanged. The summation over 'j' is then performed to obtain the conditions on the components of the physical property tensor V^m to be invariant under the group $\mathbf{C}_n$. One obtains a set of terms each of which is a product of an m-product and a trigonometric summation. The trigonometric summations are evaluated (Gradshteyn & Ryshik, 2007) to obtain conditions which are solved to determine the form of physical property tensors V^m invariant under the group $\mathbf{C}_n$. An example of this procedure is given in Appendix *B* (see supporting information).

We now discuss additional conditions on the components of the physical property tensor V^m to be invariant under line

[2] Supporting information is available from the IUCr electronic archives (Reference: XO5022).

Table 2
Limiting line point group types.

The first two columns are point group type symbols in 'Hermann–Mauguin (International)' long and short notation. The third column is in Shubnikov notation (Shubnikov, 1958, 1964), 'Hermann–Mauguin/Schoenflies' notation is in the fourth column, and a 'Schoenflies' notation is in the fifth column. The fifth column also gives the coset decomposition of the limiting line point group with respect to its subgroup $\mathbf{C}_\infty$.

Groups **G**				
∞	∞	∞	$\mathbf{C}_\infty$	$\mathbf{C}_\infty = \mathbf{C}_\infty$
∞/m	∞/m	$\infty{:}m$	$\mathbf{C}_{\infty/m}$	$\mathbf{C}_{\infty\mathrm{h}} = \mathbf{C}_\infty + \sigma_\mathrm{h}\,\mathbf{C}_\infty$
∞mm	∞m	$\infty\cdot m$	$\mathbf{C}_{\infty m}$	$\mathbf{C}_{\infty\mathrm{v}} = \mathbf{C}_\infty + \sigma_\mathrm{v}\,\mathbf{C}_\infty$
$\infty 2$	$\infty 2$	$\infty{:}2$	$\mathbf{C}_{\infty 2}$	$\mathbf{D}_\infty = \mathbf{C}_\infty + U\,\mathbf{C}_\infty$
∞/mmm	∞/mm	$m\cdot\infty{:}m$	$\mathbf{C}_{\infty/mm}$	$\mathbf{D}_{\infty\mathrm{h}} = \mathbf{C}_{\infty\mathrm{v}} + \sigma_\mathrm{h}\,\mathbf{C}_{\infty\mathrm{v}} = \mathbf{C}_\infty + \sigma_\mathrm{v}\mathbf{C}_\infty + \sigma_\mathrm{h}\,\mathbf{C}_\infty + U\,\mathbf{C}_\infty$
Groups $\mathbf{G1'}$				
$\infty 1'$	$\infty 1'$	$\underline{\infty}$	$\mathbf{C}_\infty\mathbf{1'}$	$\mathbf{C}_\infty\mathbf{1'} = \mathbf{C}_\infty + 1'\mathbf{C}_\infty$
$\infty/m1'$	$\infty/m1'$	$\underline{\infty}{:}m$	$\mathbf{C}_{\infty/m}\mathbf{1'}$	$\mathbf{C}_{\infty\mathrm{h}}\mathbf{1'} = \mathbf{C}_{\infty\mathrm{h}} + \mathbf{C}_{\infty\mathrm{h}}1' = \mathbf{C}_\infty + \sigma_\mathrm{h}\,\mathbf{C}_\infty + 1'(\mathbf{C}_\infty + \sigma_\mathrm{h}\,\mathbf{C}_\infty)$
$\infty mm1'$	$\infty m1'$	$\underline{\infty}\cdot m$	$\mathbf{C}_{\infty m}\mathbf{1'}$	$\mathbf{C}_{\infty\mathrm{v}}\mathbf{1'} = \mathbf{C}_{\infty\mathrm{v}} + \mathbf{C}_{\infty\mathrm{v}}1' = \mathbf{C}_\infty + \sigma_\mathrm{v}\,\mathbf{C}_\infty + 1'(\mathbf{C}_\infty + \sigma_\mathrm{v}\,\mathbf{C}_\infty)$
$\infty 21'$	$\infty 21'$	$\underline{\infty}{:}2$	$\mathbf{C}_{\infty 2}\mathbf{1'}$	$\mathbf{D}_\infty\mathbf{1'} = \mathbf{D}_\infty + \mathbf{D}_\infty 1' = \mathbf{C}_\infty + U\,\mathbf{C}_\infty + 1'(\mathbf{C}_\infty + U\,\mathbf{C}_\infty)$
$\infty/mmm1'$	$\infty/mm1'$	$m\cdot\underline{\infty}{:}m$	$\mathbf{C}_{\infty/mm}\mathbf{1'}$	$\mathbf{D}_{\infty\mathrm{h}}\mathbf{1'} = \mathbf{D}_{\infty\mathrm{h}} + \mathbf{D}_{\infty\mathrm{h}}1' = \mathbf{C}_\infty + \sigma_\mathrm{v}\,\mathbf{C}_\infty + \sigma_\mathrm{h}\,\mathbf{C}_\infty + U\,\mathbf{C}_\infty + 1'(\mathbf{C}_\infty + \sigma_\mathrm{v}\,\mathbf{C}_\infty + \sigma_\mathrm{h}\mathbf{C}_\infty + U\,\mathbf{C}_\infty)$
Groups $\mathbf{G}(\mathbf{H})$				
∞/m'	∞/m'	$\infty{:}\underline{m}$	$\mathbf{C}_{\infty/m}(\mathbf{C}_\infty)$	$\mathbf{C}_{\infty\mathrm{h}}(\mathbf{C}_\infty) = \mathbf{C}_\infty + \sigma_\mathrm{h}'\,\mathbf{C}_\infty$
$\infty m'm'$	$\infty m'$	$\infty\cdot\underline{m}$	$\mathbf{C}_{\infty m}(\mathbf{C}_\infty)$	$\mathbf{C}_{\infty\mathrm{v}}(\mathbf{C}_\infty) = \mathbf{C}_\infty + \sigma_\mathrm{v}'\,\mathbf{C}_\infty$
$\infty 2'$	$\infty 2'$	$\infty{:}\underline{2}$	$\mathbf{C}_{\infty 2}(\mathbf{C}_\infty)$	$\mathbf{D}_\infty(\mathbf{C}_\infty) = \mathbf{C}_\infty + U'\mathbf{C}_\infty$
$\infty/mm'm'$	∞/mm'	$\underline{m}\cdot\infty{:}m$	$\mathbf{C}_{\infty/mm}(\mathbf{C}_{\infty/m})$	$\mathbf{D}_{\infty\mathrm{h}}(\mathbf{C}_{\infty\mathrm{h}}) = \mathbf{C}_{\infty\mathrm{h}} + \sigma_\mathrm{v}'\,\mathbf{C}_{\infty\mathrm{h}} = \mathbf{C}_\infty + \sigma_\mathrm{h}\,\mathbf{C}_\infty + \sigma_\mathrm{v}'(\mathbf{C}_\infty + \sigma_\mathrm{h}\,\mathbf{C}_\infty)$
$\infty/m'mm$	$\infty/m'm$	$m\cdot\infty{:}\underline{m}$	$\mathbf{C}_{\infty/mm}(\mathbf{C}_{\infty m})$	$\mathbf{D}_{\infty\mathrm{h}}(\mathbf{C}_{\infty\mathrm{v}}) = \mathbf{C}_{\infty\mathrm{v}} + \sigma_\mathrm{h}'\,\mathbf{C}_{\infty\mathrm{v}} = \mathbf{C}_\infty + \sigma_\mathrm{v}\,\mathbf{C}_\infty + \sigma_\mathrm{h}'(\mathbf{C}_\infty + \sigma_\mathrm{v}\,\mathbf{C}_\infty)$
$\infty/m'm'm'$	$\infty/m'm'$	$\underline{m}\cdot\infty{:}\underline{m}$	$\mathbf{C}_{\infty/mm}(\mathbf{C}_{\infty 2})$	$\mathbf{D}_{\infty\mathrm{h}}(\mathbf{D}_\infty) = \mathbf{D}_\infty + \sigma_\mathrm{h}'\,\mathbf{D}_\infty = \mathbf{C}_\infty + U\,\mathbf{C}_\infty + \sigma_\mathrm{h}'(\mathbf{C}_\infty + U\,\mathbf{C}_\infty)$

point groups. Each line point group, see Table 1, can be written as a coset decomposition with respect to the group $\mathbf{C}_n$:

$$\text{line point group} = r_1\mathbf{C}_n + r_2\mathbf{C}_n + r_3\mathbf{C}_n + \ldots + r_p\mathbf{C}_n, \qquad (7)$$

where $r_1 = 1$ and r_i, $i = 1, 2, \ldots, p$, are the coset representatives of the coset decomposition. All conditions due to the invariance requirements under $\mathbf{C}_n$ on the components of the tensor V^m are provided by equation (5) and the additional conditions provided by equation (1) using the coset representatives r_i, $i = 2, \ldots, p$, of the coset decomposition [equation (7)]. For example, all conditions on the components of the tensor V^m invariant under a line point group of the family $\mathbf{D}_n$ for a specific value of n are given by the conditions due to the group $\mathbf{C}_n$ and an additional condition, equation (1), due to the coset representatives U, a twofold rotation perpendicular to the rotation axis of $\mathbf{C}_n$. This same procedure is used to determine the form of all mth ranked tensors V^m, eV^m, aV^m and aeV^m invariant under line point groups for finite n.

When n is infinite, we have the so-called *limiting line point groups* (Tavger, 1960; Bhagavantam & Pantulu, 1966; Krishnamurty & Gopalakrishnamurty, 1969). Notation for these limiting line point groups is given in Table 2. To determine the form of a physical property tensor invariant under a limiting line point group one can first determine the form under the limiting group $\mathbf{C}_\theta$, a group generated by an infinitesimal rotation C_θ. Determining the form of a physical property tensor V^m invariant under the limiting group $\mathbf{C}_\theta$ is analogous to determining the form of the tensor invariant under $\mathbf{C}_n$. The operator C_θ, representing a rotation which we take about the z axis, is applied to each component of the tensor. Each component of the tensor must be invariant under C_θ, giving a condition on each component analogous to equation (2):

$$m\text{-product}_s = C_\theta\,(m\text{-product}_s) \qquad (8)$$

for $s = 1, 2, \ldots, 3^m$. The action of C_θ on each component is to replace each x with $x\cos\theta - y\sin\theta$, each y with $x\sin\theta + y\cos\theta$, and each z is left as is. Both sides are multiplied by $\mathrm{d}\theta$ and then integrated over all angles θ from 0 to 2π to obtain conditions on the components of the tensor:

$$2\pi(m\text{-product}_s) = \int\limits_{\theta=0}^{\theta=2\pi} C_\theta\,(m\text{-product}_s)\,\mathrm{d}\theta \qquad (9)$$

for $s = 1, 2, \ldots, 3^m$. Additional conditions on the form of a physical property tensor V^m invariant under the limiting line point group are provided by equation (1) using the coset representatives, see Table 2, of the limiting line point group in the coset decomposition with respect to $\mathbf{C}_\theta$. The same procedure is used to determine the form of all mth ranked tensors V^m, eV^m, aV^m and aeV^m invariant under limiting line point groups. An example of this procedure is given in Appendix *C* (see supporting information).

3. Bypass theorem

The following theorem

The form of a physical property tensor V^m invariant under a group C_n, with $n > m$, is independent of n.

is a corollary of Hermann's theorem (Hermann, 1934) which states if an m-rank tensor has an n-fold symmetry axis and $n > m$, the tensor also has a symmetry axis of an infinite order. The proof which we shall give here is related to the methodology of the previous section, of determining the form of tensors invariant under individual finite and infinite (limiting) line point groups, and is by showing that when $n > m$ all conditions on the components of the tensor V^m, which determine the form of the tensor, are independent of n. To be invariant under

$\mathbf{C}_n$, the components of the tensor V^m must satisfy equation (5). The action of an operator $(C_n)^j$ is given by equations (6*a*), (6*b*). Consequently, the right-hand side of equation (5) becomes a set of linear terms each of which is a product of an *m*-product and a summation of the form

$$\sum_{j=1}^{n} \cos^a \frac{2\pi}{n} j \sin^b \frac{2\pi}{n} j,$$

where $a + b = s \leq m$. We shall show that for $n > m$ each of these summations is either zero or proportional to n and consequently the right-hand side of each equation (5) is either zero or proportional to n. In the former case, the *m*-product on the left-hand side of the equation is zero and in the latter, the n's cancel out. In both cases the condition on the component of the tensor is independent of n. QED

We shall prove then that with $s \leq m$, $0 \leq b \leq s$ and $n > m$

$$\sum_{j=1}^{n} \cos^{s-b} \frac{2\pi}{n} j \sin^b \frac{2\pi}{n} j = 0$$

or

$$\sum_{j=1}^{n} \cos^{s-b} \frac{2\pi}{n} j \sin^b \frac{2\pi}{n} j \propto n,$$

i.e. is equal to zero or proportional to n. The proof, given in Appendix *D* (see supporting information), is divided into eight parts depending on the value and parity of the exponents of the trigonometric functions. A summary of the results is given in Table 3.

The above theorem can be generalized to include all line point groups:

The form of a physical property tensor V^m invariant under a line point group which contains the subgroup C_n, with $n > m$, is independent of n.

The proof is based on the fact that $\mathbf{C}_n$ is a subgroup in all line point groups, see Table 1, and the coset representatives of the coset decomposition of each line group with respect to the group $\mathbf{C}_n$ give rise to additional conditions on the form of the physical property tensor which, for $n > m$, are also independent of n. For the remaining six classes of line groups of type I:

(i) For groups $\mathbf{C}_{n\mathrm{v}} = \mathbf{C}_n + \sigma_\mathrm{v}\, \mathbf{C}_n$. The form of V^m invariant under $\mathbf{C}_n$ is the same for all $n > m$. Taking $\sigma_\mathrm{v} = m_y$ for all n, which gives an additional condition independent of n, the form of V^m invariant under $\mathbf{C}_{n\mathrm{v}}$ is then the same for all $n > m$.

(ii) For groups $\mathbf{S}_{2n} = \mathbf{C}_n + (\sigma_\mathrm{h} C_{2n})\, \mathbf{C}_n$. The form of V^m invariant under $\mathbf{C}_n$ is the same for all $n > m$. It is then also invariant under $\mathbf{C}_{2n}$, since $2n > n > m$, and therefore in particular under the element C_{2n}. The element σ_h gives rise to a condition that causes all components with one or three z's to be zero, a condition independent of n. The form of V^m invariant under $\mathbf{S}_{2n}$ is then the same for all $n > m$.

(iii) For groups $\mathbf{C}_{n\mathrm{h}} = \mathbf{C}_n + \sigma_\mathrm{h}\, \mathbf{C}_n$. The form of V^m invariant under $\mathbf{C}_n$ is the same for all $n > m$. The element σ_h gives rise to a condition independent of n. The form of V^m invariant under $\mathbf{C}_{n\mathrm{h}}$ is then the same for all $n > m$.

Table 3
Value of trigonometric summations $\sum_{j=1}^{n} \cos^{s-b}(2\pi/n)j \sin^b(2\pi/n)j$ in conditions on components of tensors V^m invariant under groups $\mathbf{C}_n$, $n > m$, with $s \leq m$ and $0 \leq b \leq s$.

s even:

$$\sum_{j=1}^{n} \cos^s \frac{2\pi}{n} j \propto n \qquad \sum_{j=1}^{n} \sin^s \frac{2\pi}{n} j \propto n$$

s odd:

$$\sum_{j=1}^{n} \cos^s \frac{2\pi}{n} j = 0 \qquad \sum_{j=1}^{n} \sin^s \frac{2\pi}{n} j = 0$$

$b \neq 0$ or s and even, $s - b$ even and s even:

$$\sum_{j=1}^{n} \cos^{s-b} \frac{2\pi}{n} j \sin^b \frac{2\pi}{n} j = 0 \text{ or } \propto n$$

$b \neq 0$ or s and odd, $s - b$ even and s odd:

$$\sum_{j=1}^{n} \cos^{s-b} \frac{2\pi}{n} j \sin^b \frac{2\pi}{n} j = 0$$

$b \neq 0$ or s and odd, $s - b$ odd and s even:

$$\sum_{j=1}^{n} \cos^{s-b} \frac{2\pi}{n} j \sin^b \frac{2\pi}{n} j = 0$$

$b \neq 0$ or s and even, $s - b$ odd and s odd:

$$\sum_{j=1}^{n} \cos^{s-b} \frac{2\pi}{n} j \sin^b \frac{2\pi}{n} j = 0$$

(iv) For groups $\mathbf{D}_n = \mathbf{C}_n + U\, \mathbf{C}_n$. The form of V^m invariant under $\mathbf{C}_n$ is the same for all $n > m$. Taking $U = 2_x$ for all n, the form of V^m invariant under $\mathbf{D}_n$ is then the same for all $n > m$.

(v) For groups $\mathbf{D}_{nd} = \mathbf{C}_{n\mathrm{v}} + U_d\, \mathbf{C}_{n\mathrm{v}}$. The form of V^m invariant under $\mathbf{C}_{n\mathrm{v}}$ is the same for all $n > m$. We take $\sigma_\mathrm{v} = m_y$ for all n and rotate the coordinate system through an angle of $\pi/2n$. The form of V^m is also invariant under the operation C_{4n}, since $4n > n > m$, and we now take a rotation $U_d = U_y$ along the new y axis for all $n > m$. The form of V^m invariant under $\mathbf{D}_{nd}$ is then the same for all $n > m$.

(vi) For groups $\mathbf{D}_{n\mathrm{h}} = \mathbf{C}_{n\mathrm{v}} + \sigma_\mathrm{h}\, \mathbf{C}_{n\mathrm{v}}$. The form of V^m invariant under $\mathbf{C}_{n\mathrm{v}}$ is the same for all $n > m$. The element σ_h gives rise to a condition independent of n. The form of V^m invariant under $\mathbf{D}_{n\mathrm{h}}$ is then the same for all $n > m$.

For the remaining line point groups of types II and III, see Table 1, proofs are analogous to those given for the above line point groups since the action of the time inversion operation $1'$ on components of a tensor V^m is independent of n. As actions of all elements of line point groups on both tensors e and a are independent of the value of n, the preceding theorem and corollary are also valid for physical property tensors eV^m, aV^m and aeV^m. This then gives the general form of the above theorem which we shall refer to as the *Bypass theorem*:

The form of physical property tensors V^m, eV^m, aV^m and aeV^m invariant under a line point group which contains the

Table 4
Finite line group families to limiting line point group type as $n \to \infty$.

Groups **G**		
$\mathbf{C}_n$	$\to$	$\mathbf{C}_\infty$
$\mathbf{C}_{n\mathrm{v}}$	$\to$	$\mathbf{C}_{\infty\mathrm{v}}$
$\mathbf{C}_{n\mathrm{h}}$, $\mathbf{S}_{2n}$	$\to$	$\mathbf{C}_{\infty\mathrm{h}}$
$\mathbf{D}_n$	$\to$	$\mathbf{D}_\infty$
$\mathbf{D}_{n\mathrm{h}}$, $\mathbf{D}_{nd}$	$\to$	$\mathbf{D}_{\infty\mathrm{h}}$
Groups **G1′**		
$\mathbf{C}_n\mathbf{1}'$	$\to$	$\mathbf{C}_\infty\mathbf{1}'$
$\mathbf{C}_{n\mathrm{v}}\mathbf{1}'$	$\to$	$\mathbf{C}_{\infty\mathrm{v}}\mathbf{1}'$
$\mathbf{C}_{n\mathrm{h}}\mathbf{1}'$, $\mathbf{S}_{2n}\mathbf{1}'$	$\to$	$\mathbf{C}_{\infty\mathrm{h}}\mathbf{1}'$
$\mathbf{D}_n\mathbf{1}'$	$\to$	$\mathbf{D}_\infty\mathbf{1}'$
$\mathbf{D}_{n\mathrm{h}}\mathbf{1}'$, $\mathbf{D}_{nd}\mathbf{1}'$	$\to$	$\mathbf{D}_{\infty\mathrm{h}}\mathbf{1}'$
Groups **G**(**H**)		
$\mathbf{C}_{2n}(\mathbf{C}_n)$	$\to$	$\mathbf{C}_\infty\mathbf{1}'$
$\mathbf{S}_{2n}(\mathbf{C}_n)$, $\mathbf{C}_{n\mathrm{h}}(\mathbf{C}_n)$	$\to$	$\mathbf{C}_{\infty\mathrm{h}}(\mathbf{C}_\infty)$
$\mathbf{C}_{2n\mathrm{h}}(\mathbf{S}_{2n})$, $\mathbf{C}_{2n\mathrm{h}}(\mathbf{C}_{n\mathrm{h}})$	$\to$	$\mathbf{C}_{\infty\mathrm{h}}\mathbf{1}'$
$\mathbf{D}_n(\mathbf{C}_n)$	$\to$	$\mathbf{D}_\infty(\mathbf{C}_\infty)$
$\mathbf{D}_{2n}(\mathbf{D}_n)$	$\to$	$\mathbf{D}_\infty\mathbf{1}'$
$\mathbf{C}_{n\mathrm{v}}(\mathbf{C}_n)$	$\to$	$\mathbf{C}_{\infty\mathrm{v}}(\mathbf{C}_\infty)$
$\mathbf{C}_{2n\mathrm{v}}(\mathbf{C}_{n\mathrm{v}})$	$\to$	$\mathbf{C}_{\infty\mathrm{v}}\mathbf{1}'$
$\mathbf{D}_{nd}(\mathbf{D}_n)$, $\mathbf{D}_{n\mathrm{h}}(\mathbf{D}_n)$	$\to$	$\mathbf{D}_{\infty\mathrm{h}}(\mathbf{D}_\infty)$
$\mathbf{D}_{nd}(\mathbf{C}_{n\mathrm{v}})$, $\mathbf{D}_{n\mathrm{h}}(\mathbf{C}_{n\mathrm{v}})$	$\to$	$\mathbf{D}_{\infty\mathrm{h}}(\mathbf{C}_{\infty\mathrm{v}})$
$\mathbf{D}_{nd}(\mathbf{C}_{n\mathrm{h}})$, $\mathbf{D}_{nd}(\mathbf{S}_{2n})$	$\to$	$\mathbf{D}_{\infty\mathrm{h}}(\mathbf{C}_{\infty\mathrm{h}})$
$\mathbf{D}_{2n\mathrm{h}}(\mathbf{D}_{nd})$, $\mathbf{D}_{2n\mathrm{h}}(\mathbf{D}_{n\mathrm{h}})$	$\to$	$\mathbf{D}_{\infty\mathrm{h}}\mathbf{1}'$

subgroup C_n, with $n > m$, is invariant under the limiting group of that line point group.

The limiting group family of each line point group family as $n \to \infty$ is given in Table 4.

As a consequence of this Bypass theorem, if one is to determine the form of an mth rank tensor invariant under all line point groups, one needs only to determine the form of the tensor for those line point groups with $n = 1, 2, \ldots, m$ and $n = \infty$. The form of the tensor for all $n > m$ is the same as for $n = \infty$.

4. Physical property tensors of rank two invariant under line point groups

We consider all physical property tensors of rank two and internal symmetries as considered by Sirotin & Shaskolskaya (1982); in terms of Jahn symbols these are the 12 tensors

$$\begin{array}{cccc} V^2 & eV^2 & aV^2 & aeV^2 \\ [V^2] & e[V^2] & a[V^2] & ae[V^2] \\ \{V^2\} & e\{V^2\} & a\{V^2\} & ae\{V^2\}, \end{array} \quad (10)$$

where $[V^2]$ denotes that the tensor is symmetrized, *i.e.* $V_{ij} = V_{ji}$, and $\{V^2\}$ that the tensor is anti-symmetrized, *i.e.* $V_{ij} = -V_{ji}$. Among these physical property tensors are, *e.g.*, tensors of: dielectric, magnetic and toroidic susceptibility $[V^2]$; electrotoroidic coefficients aV^2; magnetotoroidic coefficients and gyration eV^2; and magnetoelectric coefficients aeV^2.

The infinite number of line point groups of each family of line point groups are indexed by an index $n = 1, 2, \ldots, \infty$. Using the Bypass theorem, for each of these rank-two tensors, to tabulate the form of the tensor invariant under the infinity of line point groups of each line point group family, one needs only to list the form of the tensor for representative line groups of three line group types, for representative line point groups indexed by $n = 1$, 2 and ∞. The form of each tensor invariant under a line point group indexed by a value of $n > 2$ is the same as the form of the tensor invariant under the line point group of that family indexed by $n = \infty$. The form of these tensors for a representative line point group of each of the three types in each line group family is given in Table 5 (see supporting information). Subsets of this table can be found in the works of Milošević (1995), Dmitriev (2003) and Sirotin & Shaskolskaya (1982).

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