# Integral Rational Bases of Tensor Invariants of Crystallographic Groups

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**Abstract**

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# Integral Rational Bases of Tensor Invariants of Crystallographic Groups

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**1.** Tensor invariants of a crystallographic group are polynomials composed of the components of one or several tensors and invariant with respect to this group. They are used in expanding thermodynamic functions of state of crystals into series, in constructing tensors invariant with respect to crystallographic groups, etc. As is known (1), all invariants of one or several tensors can be obtained by integral rational operations—multiplication and linear combination—from a finite set of such invariants, called their integral rational basis (i.r.b.). For crystallographic groups, i.r.b.' s of vector invariants (2) and i.r.b.' s of invariants of a symmetric tensor of the second rank (3) are known. Here a general method is set forth for constructing i.r.b.'s of tensor invariants of crystallographic groups —a generalization of a method proposed earlier for constructing tensors invariant with respect to crystallographic groups (4).

**2.** For definiteness, we shall consider two tensors $\vec{\alpha}$ and $\vec{\beta}$, whose components transform respectively according to a representation $A$ of the orthogonal group of dimension $a$ and according to its representation $B$ of dimension $b$. Polynomials composed of their components, of degree $m$ in the components of the tensor $\vec{\alpha}$ and of degree $n$ in the components of the tensor $\vec{\beta}$, transform according to the representation[*] $T = [A^m][B^n]$. In the linear space $L(T)$ of such polynomials, the invariants of the crystallographic group $G$ form a subspace $L(G \times T)$. The averaging operators (cf. (4))

$$\hat{S}(G \times T) = \frac{1}{N_G} \sum_{g \in G} \hat{T}(g),$$

where $N_G$ is the order of the group $G$, and $\hat{T}(g)$ is the operator of the representation $T$ of the group $G$ corresponding to the element $g$, map the space $L(T)$ onto its subspace $L(G \times T)$.

**3.** We shall agree to use in $L(T)$ bases consisting of all possible monomials

$$\alpha_1^{s_1} \alpha_2^{s_2} \ldots \alpha_a^{s_a} \beta_1^{t_1} \beta_2^{t_2} \ldots \beta_b^{t_b} \left( \sum_{i=1}^{a} s_i = m, \ \sum_{j=1}^{b} t_j = n \right).$$

In doing so, if we seek an i.r.b. of invariants of groups of the lower or cubic systems, we shall write the tensors $\vec{\alpha}$ and $\vec{\beta}$ in the orthogonal crystallophysical (${}^5$) coordinate system $x, y, z$. If, however, it is required to find an i.r.b. of invariants of groups of the middle systems, we shall write the tensors $\vec{\alpha}$ and $\vec{\beta}$ in the cyclic (${}^6$) coordinate system $\xi, \eta, z$, obtained from the crystallophysical one by the unitary transformation

$$\xi = 2^{-1/2}(x+iy), \quad \eta = 2^{-1/2}(x-iy).$$

**4.** Suppose first that the representation $T$ of the group $G$ splits into one-dimensional representations. For this it is sufficient (and if $T$ is a faithful representation, also necessary) that the group $G$ be Abelian. In this case, the bases chosen in Sec. 3 in the space $L(T)$ consist of eigenvectors of the operators $\hat{T}(g)$. The action of the operator $\hat{S}$ on the elements of such a basis reduces to selecting monomials, i.e., to multiplying the monomials satisfying certain "selection rules" by one and multiplying the remaining basis monomials by zero. Further, as in (4), we easily find an i.r.b. of the selected monomials for all possible $T = [A^m][B^n]$ $(m, n = 0, 1, 2, \ldots)$.

5. Let us explain the foregoing by an example. We shall find an i.r.b. of the invariants of a vector $\vec{\alpha} = (A = V)$ and a pseudovector $\vec{\beta}$ $(B = \varepsilon V)$ with respect to the group $D_{2h}$. The basis in $L(T)$ consists of all possible monomials of the form

$$\alpha_x^{s_x}\alpha_y^{s_y}\alpha_z^{s_z}\beta_x^{t_x}\beta_y^{t_y}\beta_z^{t_z} \qquad (s_x+s_y+s_z=m,\ t_x+t_y+t_z=n).$$

The group-averaging operator over the group $D_{2h}$, referred to this basis, is:

$$\begin{aligned}\hat{S}\,(D_{2h}\times[V^m][(\varepsilon V)^n]) &= \frac{1}{8}[1+(-1)^{m-s_x+n-t_x}+(-1)^{m-s_y+n-t_y}\\ &\quad+(-1)^{m-s_z+n-t_z}+(-1)^m+(-1)^{s_x+n-t_x}\\ &\quad+(-1)^{s_y+n-t_y}+(-1)^{s_z+n-t_z}]\\ &=\begin{cases}1, & \text{if } s_x+t_x\equiv s_y+t_y\equiv s_z+t_z \pmod 2,\ m\equiv 0 \pmod 2;\\ 0, & \text{in all other cases.}\end{cases}\end{aligned}$$

Hence, as in (4), we find an i.r.b. consisting of the following 13 invariants:

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[*] The symbol $[A^m]$ denotes the $m$-th symmetric Kronecker power of the representation $A$, in distinction to the ordinary Kronecker power, denoted by $A^m$.

$$\begin{gathered}I_1 = \alpha_x^2, \qquad I_2 = \alpha_y^2, \qquad I_3 = \alpha_z^2, \\ J_1 = \beta_x^2, \qquad J_2 = \beta_y^2, \qquad J_3 = \beta_z^2, \qquad K = \beta_x\beta_y\beta_z, \\ L_1 = \alpha_y\alpha_z\beta_x, \qquad L_2 = \alpha_z\alpha_x\beta_y, \qquad L_3 = \alpha_x\alpha_y\beta_z, \\ M_1 = \alpha_y\alpha_z\beta_y\beta_z, \qquad M_2 = \alpha_z\alpha_x\beta_z\beta_x, \qquad M_3 = \alpha_x\alpha_y\beta_x\beta_y.\end{gathered}$$

The invariants $I_p$, consisting only of the components of $\vec{\alpha}$, form an i.r.b. of the invariants of a vector, coinciding with that indicated in (2). Similarly, the invariants $J_q$ and $K$ form an i.r.b. of the invariants of a pseudovector with respect to the group $D_{2h}$. Among the 13 invariants listed, 6 are functionally independent (say, $I_p$ and $J_q$). The remaining ones are related to them and to one another by 28 relations***:

$$\begin{gathered}K^2 = J_1J_2J_3, \qquad L_1^2 = I_2I_3J_1, \qquad M_1^2 = I_2I_3J_2J_3, \\ L_2L_3 = I_1M_1, \qquad M_2M_3 = I_1J_1M_1, \qquad KL_1 = J_1M_1, \qquad KM_1 = J_2J_3M_1, \\ L_1M_1 = I_2I_3K, \qquad L_2M_3 = I_1J_2L_1, \qquad L_3M_2 = I_1J_3L_1\end{gathered}$$

(among them, of course, only 7 are functionally independent). Taking these relations into account, we refine, following Smith (8), the form of the general integral rational invariant of the group $D_{2h}$, composed of the components of the vectors $\vec{\alpha}$ and $\vec{\beta}$. Obviously, any such invariant, i.e. any polynomial in the 13 basic invariants, can be written in the following form:

$$P(I_p, J_q, K, L_r, M_s) = f + K\varphi + \sum_{r=1}^{3} L_r\psi_r + \sum_{s=1}^{3} M_s\chi_s,$$

where $f, \varphi, \psi_r, \chi_s$ are arbitrary polynomials in the six principal (functionally independent) invariants $I_p, J_q$.

6. To construct an i.r.b. of invariants of non-Abelian crystallographic groups, we shall use the easily proved theorem on averaging over subgroups. Let $F$ and $H$ be subgroups of a group $G$ having no common elements except the identity, and let the product of their orders be equal to the order of the group $G$; then, for any $T$,

$$\hat{S}(G \times T) = \hat{S}(F \times T)\hat{S}(H \times T) = \hat{S}(H \times T)\hat{S}(F \times T).$$

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* $V$ is the vector representation, $\varepsilon$ is the pseudoscalar representation.

** More precisely, with respect to the supergroup (7) $D_{2h}$: the i.r.b.' s of the invariants of a pseudovector are the same with respect to the other groups belonging to this supergroup, $C_{2v}$ and $D_2$.

*** To each of the written relations (except the first) there correspond two more, obtained from it by a cyclic permutation of the indices.

For every non-Abelian crystallographic group $G$ one can choose subgroups $F$ and $H$, satisfying the conditions of this theorem, in such a way that $F$ is Abelian, while $H$ is isomorphic to the symmetric group of degree three or to one of its subgroups. Moreover, the bases indicated in Sec. 3 in $L(T)$ are chosen so that the operators $\hat{T}(h)$ of the representation $T$ of the group $H$ perform permutations of indices in the basis monomials (sometimes, in addition, they change the signs of monomials). Hence there follows a method for constructing an i.r.b. of invariants of the non-Abelian group $G$. First, as shown in Sec. 4, we find an i.r.b. of invariants of its Abelian subgroup $F$. The next stage of the problem reduces to constructing an i.r.b. of invariants of the symmetric or signed-permutation group of degree three or two, described, for example, in ($^1$). One may, of course, proceed in the reverse order as well.

7. Let us consider this case in a simpler example. Let $\vec{\alpha}$ be, as before, a vector ($A = V$), and let $\beta$ be a pseudoscalar or a tensor of rank three antisymmetric in all indices ($B = \varepsilon$), with $\gamma = \beta_{xyz}$ in a right-handed coordinate system. We shall find an i.r.b. of invariants of these tensors with respect to the cubic groups. We choose the subgroups $F$ and $H$ of the cubic groups $G$ as follows:

| $G$ | $T$ | $T_h$ | $T_d$ | $O$ | $O_h$ |
|---|---|---|---|---|---|
| $F$ | $D_2$ | $D_{2h}$ | $D_2$ | $D_2$ | $D_{2h}$ |
| $H$ | $C_3$ | $C_3$ | $C_{3v}$ | $D_3$ | $C_{3v}$ |

An i.r.b. for the group $D_2$ consists of the invariants $\alpha_x^2, \alpha_y^2, \alpha_z^2, \xi = \alpha_x\alpha_y\alpha_z$, and $\beta$, while for the group $D_{2h}$ it consists of the invariants $\alpha_x^2, \alpha_y^2, \alpha_z^2, \beta^2$, and $\xi\beta$. Averaging over the groups $H$ reduces to constructing from these invariants symmetric polynomials or polynomials invariant with respect to a signed-permutation group, taking into account that under certain operations $\beta$ and $\xi\beta$ change sign. Introducing the notation

$$\alpha^2 = \alpha_x^2 + \alpha_y^2 + \alpha_z^2, \qquad \gamma^2 = \alpha_x^4 + \alpha_y^4 + \alpha_z^4,$$

$$\eta = (\alpha_x^2 - \alpha_y^2)(\alpha_y^2 - \alpha_z^2)(\alpha_z^2 - \alpha_x^2),$$

we easily obtain the following i.r.b.' s:

Group $T$: $\alpha^2, \xi, \gamma^2, \eta, \beta$;

Group $T_h$: $\alpha^2, \gamma^2, \xi^2, \eta, \beta^2, \xi\beta$;

Group $T_d$: $\alpha^2, \xi, \gamma^2, \beta^2$;

Group $O$: $\alpha^2, \gamma^2, \xi^2, \xi\eta, \beta$;

Group $O_h$: $\alpha^2, \gamma^2, \xi^2, \beta^2$.

In those cases where there are more than four basic invariants, there exist relations among them by means of which, as in Sec. 5, one can refine the form of the general invariant composed of the components of the tensors $\alpha$ and $\beta$.

For the group $T$ we thus obtain:

$$P(\alpha^2, \xi, \gamma^2, \eta, \beta) = f_1(\alpha^2, \xi, \gamma^2, \beta) + \eta f_2(\alpha^2, \xi, \gamma^2, \beta);$$

for the group $T_h$:

$$\begin{gathered}P(\alpha^2, \gamma^2, \xi^2, \eta, \beta^2, \xi\beta) = f_1(\alpha^2, \gamma^2, \xi^2, \beta^2) + \eta f_2(\alpha^2, \gamma^2, \xi^2, \beta^2) \\ +\xi\beta f_3(\alpha^2, \gamma^2, \xi^2, \beta^2) + \eta\xi\beta f_4(\alpha^2, \gamma^2, \xi^2, \beta^2);\end{gathered}$$

for the group $O$:

$$P(\alpha^2, \gamma^2, \xi^2, \xi\eta, \beta) = f_1(\alpha^2, \gamma^2, \xi^2, \beta) + \xi\eta f_2(\alpha^2, \gamma^2, \xi^2, \beta),$$

where $f_1, f_2, f_3, f_4$ are arbitrary polynomials in their four arguments—the principal invariants of the corresponding groups.

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*Note: Figure translations are in progress. See original paper for figures.*