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Extended integrity bases of irreducible matrix groups—the crystal point groups

Vojtěch Kopský

Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, POB 24, 180 40 Praha 8, Czechoslovakia

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Abstract. Any extended integrity basis (EIB) of a finite group can be composed from EIBs of irreducible matrix groups defined by irreducible representations of the group in question. The EIBs thus defined for irreducible matrix groups relevant to crystal point groups (and in virtue also to magnetic point groups) are derived with the use of a previously reported algorithm based on the successive use of Clebsch–Gordan reductions. The EIBs of vector representation of crystal point groups are derived with the use of these fundamental EIBs. Division of invariants into denominator and numerator invariants enables one to find a general functional expression of an invariant or covariant with the use of EIBs. A possible approach to phase transition theory which goes beyond the usual Landau (polynomial) approximation is given to illustrate the use of EIBs.

1. Introduction

Functions which transform by ireps (irreducible representations) of physical groups of symmetry are necessary in the consideration of classical as well as of quantum mechanical models of symmetric systems. Here we shall consider the calculation of such functions for the ordinary and magnetic crystal point groups in quite a general form. It is well known that systems of polynomial invariants are generated by finite sets called integrity bases if the group is finite. The latter have been considered, for the crystal point groups, in a number of works and in various contexts (Döring 1958, Smith *et al* 1963, Smith and Rivlin 1964, Spencer 1971, Killingbeck 1972, McLellan 1974, Kopský 1975, Patera and Winternitz 1975, Bickerstaff and Wybourne 1976). Polynomial covariants (the term introduced by Weyl (1946) which we prefer to the more usual symmetry-adapted basis) in three-dimensional vector coordinates (x, y, z)—harmonics—have been considered in a large number of papers, starting with Bethe (1929), von der Lage and Bethe (1947), Bell (1954), Altmann (1957) to name a few, and referring for a more complete list to the monograph by Bradley and Cracknell (1972).

The calculation of various kinds of polynomial and tensorial covariants can be most conveniently performed with the use of successive Clebsch–Gordan (CG) reductions. To standardise the calculations we gave, for crystal point groups, tables of so-called CG products (Kopský 1976a, b) from which one can directly read how to multiply covariants of different types. The use of these tables is far easier than the use of ordinary tables of CG coefficients (Koster *et al* 1963). We have used them already for the calculation of tensorial covariants for the ordinary and magnetic point groups (Kopský 1979a, b), and here we shall use them for the construction of extended integrity bases (EIBs). We have discussed the general problem of the construction of EIBs for polynomial algebras on which there acts a finite group G in a previous paper (Kopský 1979c, hereafter referred to as I). It turns out that covariants form linear spaces of infinite dimensions, but that these spaces are generated by finite sets of covariants called 'linear integrity bases' (McLellan 1974, Kopský 1975, Patera *et al* 1978) in the sense that any covariant is a linear combination of basic covariants with invariants as coefficients of combination. Together with the integrity bases of invariants we call these sets the EIBs.

It has also been shown in I that all EIBs of a given group G can be constructed from fundamental EIBs of algebras defined on sets of variables belonging to single ireps of this group—the typical EIBs in the language of our work (Kopský 1976a, b). We shall amplify this result somewhat; it will be shown that fundamental EIBs are those which are defined by irreducible matrix groups. We shall then derive and tabulate the EIBs of irreducible matrix groups defined by ireps of crystal point groups (they are the same as for magnetic point groups). As an example of the use of EIBs we shall consider a possible generalisation of Landau (polynomial and truncated) potentials in the theory of structural phase transitions.

2. Factorisation of polynomial algebra—the typical algebras

Generally we consider a group G acting on a G-module L_n, so that $g\boldsymbol{x} \in L_n$. Relation $gp(\boldsymbol{x}) = p(g^{-1}\boldsymbol{x})$ extends the operation of G on the algebra $\mathscr{P}(L_n)$ of polynomials $p(\boldsymbol{x})$, $\boldsymbol{x} \in L_n$. The original G-module L_n splits into minimal $\chi_\alpha(G)$-modules $L_{\alpha a}$,

$$L_n = \bigoplus_{\alpha=1}^{\kappa} \bigoplus_{a=1}^{n_\alpha} L_{\alpha a}, \tag{1}$$

and accordingly the algebra $\mathscr{P}(L_n)$ can be factorised into a direct product of its subalgebras $\mathscr{P}(L_{\alpha a})$:

$$\mathscr{P}(L_n) = \bigotimes_{\alpha=1}^{\kappa} \bigotimes_{a=1}^{n_\alpha} \mathscr{P}(L_{\alpha a}). \tag{2}$$

An EIB of the algebra $\mathscr{P}(L_n)$ consists of n algebraically independent invariants $I_1, I_2, \ldots, I_n$, possibly of a set of numerator invariants $E_1, E_2, \ldots, E_m$, and of sets of $\Gamma_{0\alpha}$-covariants $\boldsymbol{p}_1^{(\alpha)}, \boldsymbol{p}_2^{(\alpha)}, \ldots, \boldsymbol{p}_m^{(\alpha)}$, such that any polynomial invariant J is given by

$$J = P_0(I_j) + \sum_k P_k(I_j)E_k, \tag{3}$$

and any polynomial covariant $\boldsymbol{p}^{(\alpha)}$ is given by

$$\boldsymbol{p}^{(\alpha)} = \sum_a P_a(I_j)\boldsymbol{p}_a^{(\alpha)}. \tag{4}$$

Replacing polynomials in I_j by functions, we arrive at a functional expression for an invariant or a covariant.

All spaces $L_{\alpha a}$ are alike—operator-isomorphic (Hall 1959)—and we can consider them as copies of one typical $\chi_\alpha(G)$-module L_α. Quite analogously we conclude that all algebras $\mathscr{P}(L_{\alpha a})$ are copies of the typical algebra $\mathscr{P}(L_\alpha)$. The EIB of the typical algebra generally consists of $d_\alpha = \chi_\alpha(e) = \dim L_\alpha$ algebraically independent denominator invariants $I_1(\boldsymbol{x}^{(\alpha)})$, $I_2(\boldsymbol{x}^{(\alpha)}), \ldots, I_{d_\alpha}(\boldsymbol{x}^{(\alpha)})$, possibly of numerator invariants $E_1(\boldsymbol{x}^{(\alpha)})$, $E_2(\boldsymbol{x}^{(\alpha)}), \ldots, E_{m_\alpha}(\boldsymbol{x}^{(\alpha)})$, and of $\Gamma_{0\beta}$-covariants $\boldsymbol{p}_1^{(\beta)}(\boldsymbol{x}^{(\alpha)})$, $\boldsymbol{p}_2^{(\beta)}(\boldsymbol{x}^{(\alpha)}), \ldots, \boldsymbol{p}_{m_\alpha^\beta}^{(\beta)}(\boldsymbol{x}^{(\alpha)})$. Knowing the EIBs of typical algebras for the group G we can at once write those invariants and covariants of the EIB of any algebra $\mathscr{P}(L_n)$ which are copies of the typical ones. Among them will be all $n = \Sigma_\alpha d_\alpha n_\alpha$ denominator invariants, the copies of numerator invariants if any, and the copies of covariants. Furthermore, there will be those invariants and covariants which we obtain from the multiplication of subalgebras between themselves. Particularly, all invariants thus obtained will be the numerator invariants. To get the EIB we have to apply the CG multiplication and eliminate the reducible invariants and covariants. The procedure can be carried further: for example, the product of subalgebras $\mathscr{P}(L_{\alpha 1}) \otimes \mathscr{P}(L_{\alpha 2})$ is like the product $\mathscr{P}(L_{\alpha 1}) \otimes \mathscr{P}(L_{\alpha 3})$ and so on. In the case of abelian groups we get an exceedingly general result in the form of typical EIBs for all possible variables (Kopský 1975), and the procedure of derivation is quite clear.

Let us finally note that for the derivation of EIBs of typical algebras as well as for the further multiplication of these algebras we use one table of CG products common to all groups of a given isomorphic type.

3. Irreducible matrix groups

We can go further in simplifying the approach using the fact that, up to labelling of ireps and up to equivalence of ireps within each relevant class of them, the EIB of an algebra $\mathscr{P}(L_\alpha)$ is determined by the irreducible matrix group defined by the irep $\Gamma_{0\alpha}(G)$: $g \to D^{(\alpha)}(g)$.

Indeed, the irep $\Gamma_{0\alpha}(G)$ is a homomorphism of G onto certain group of matrices. The kernel of this homomorphism, $\ker \Gamma_{0\alpha}(G) = H_\alpha \lhd G$, is that normal subgroup H_α of G the elements of which are, in the irep $\Gamma_{0\alpha}(G)$, represented by the unit matrix I_α of dimension d_α: $D^{(\alpha)}(h) = I_\alpha$ if and only if $h \in H_\alpha$. Elements of the cosets in the factorisation $G = \Sigma_i g_i H_\alpha = \Sigma_i H_\alpha g_i$ are, in this irep, represented by the same matrices: $\gamma_i = g_i H_\alpha = H_\alpha g_i$ implies that $D^{(\alpha)}(g_i h) = D^{(\alpha)}(h g_i) = D^{(\alpha)}(\gamma_i)$ for $h \in H_\alpha$. The irep $\Gamma_{0\alpha}(G)$ is therefore a canonical epimorphism which maps the group G onto the matrix group $\Gamma_{0\alpha}(\mathscr{H}_\alpha)$, an irreducible faithful matrix irep of a group $\mathscr{H}_\alpha \approx G/H_\alpha$ isomorphic to factor group G/H_α with which we simply identify $\mathscr{H}_\alpha$.

The group $\mathscr{H}_\alpha$ has its own set of matrix ireps $\Gamma_{0\beta}(\mathscr{H}_\alpha)$ or its own typical matrix representation

$$\Gamma_0(\mathscr{H}_\alpha) = \bigoplus_{\beta=1}^{\lambda} \Gamma_{0\beta}(\mathscr{H}_\alpha).$$

Each of these ireps engenders (Jansen and Boon 1967) a matrix irep $\Gamma_{0\beta}(G)$ by assigning the same matrix $D^{(\beta)}(\gamma_i)$ to all elements of the coset $\gamma_i = g_i H_\alpha = H_\alpha g_i$. The space L_α can be considered as an $\mathscr{H}_\alpha$-module, especially the $\chi_\alpha(\mathscr{H}_\alpha)$-module, as well as a G-module, especially the $\chi_\alpha(G)$-module. Quite analogously, any $\chi_\beta(\mathscr{H}_\alpha)$-module can be considered as a $\chi_\beta(G)$-module; this is a procedure of lifting from group $\mathscr{H}_\alpha$ to group G. The algebra $\mathscr{P}(L_\alpha)$ is then an $\mathscr{H}_\alpha$-module, and as such it splits into $\chi_\beta(\mathscr{H}_\alpha)$-modules which can be described in terms of $\Gamma_{0\beta}(\mathscr{H}_\alpha)$-covariants forming the EIB. Each $\Gamma_{0\beta}(\mathscr{H}_\alpha)$-

covariant can be, however, considered as a $\Gamma_{0\beta}(G)$-covariant, the algebra $\mathscr{P}(L_\alpha)$ can be considered as a G-module, and the EIB of $\mathscr{P}(L_\alpha)$ is (maybe up to labelling) independent of whether we consider it as an $\mathscr{H}_\alpha$-module or as a G-module. In fact G may mean any group which is a normal extension (Hall 1959) of any group H_α by the factor group $\mathscr{H}_\alpha$. In practice, however, it may happen that the labelling of ireps of the group G does not coincide with the labelling of ireps of $\mathscr{H}_\alpha$, in which case correlation of labelling is necessary. An obvious conclusion from this consideration is that the polynomials on L_α generate only those $\Gamma_{0\beta}(G)$-covariants for which the irep $\Gamma_{0\beta}(G)$ is engendered by some irep $\Gamma_{0\beta}(\mathscr{H}_\alpha)$. These are just those ireps of G which are induced by the identity irep of H_α, or equivalently, as follows from the Frobenius reciprocity theorem, those which subduce the identity irep of H_α as many times as is their dimension. On the other hand, each of these ireps is generated by $\Gamma_{0\alpha}(G)$ because, as an irep $\Gamma_{0\alpha}(\mathscr{H}_\alpha)$ of the factor group $\mathscr{H}_\alpha$, the latter is faithful.

This relation is, in the theory of Molien series, reflected by the fact that

$$F_\beta(L_\alpha, \lambda_\alpha) = \frac{1}{N} \sum_{g \in G} \frac{\chi_\beta^*(g)}{\det(I_\alpha - \lambda_\alpha D^{(\alpha)}(g))}$$

is (provided the labelling is correlated) the same in G as in $\mathscr{H}_\alpha$. Indeed, the terms in the sum are all the same; in the case of group G every term appears $[G : H_\alpha]$ times ($[G : H_\alpha]$ being the index of H_α in G), but the order N of G is just $[G : H_\alpha]$ times the order of $\mathscr{H}_\alpha$. We shall illustrate the situation in § 5.

4. The crystal and magnetic point groups

It can be easily found by inspection that there are, with the exception of the trivial group $\Gamma_1(C_1)$ consisting of unity only, 12 non-equivalent irreducible matrix groups from which all ireps of crystal and magnetic point groups can be composed. In this enumeration we consider a pair of one-dimensional mutually conjugate complex ireps of cyclic groups (and of groups of Laue class T) as one physically irreducible (reducible in a complex field, but irreducible in a real field) irep because they have the same kernel and describe a doubly degenerate mode. The EIBs of these 12 irreducible matrix groups are given in table A1 of the Appendix. The calculations were performed with the use of the algorithm described in I on the basis of CG tables given by Kopský (1976a, b); the numerical labelling of ireps and the choice of matrices and symbols for typical variables are the same as in the latter work. The symbol at the left upper corner of each part of the table specifies the irreducible matrix group as a faithful matrix irep of a group of proper rotations or of a centrosymmetrical group. The first row lists the other ireps of this group and the typical variables with labelling corresponding to this group. The polynomial covariants are given in the corresponding columns; to save space we do not list the linear covariants, and the numerical labels are dropped in the polynomials. For cyclic and dihedral groups C_n, D_n we give the EIBs for two choices of typical representations—the complex and the real one. It should be mentioned that whenever we join two conjugate complex ireps $\Gamma_{0\gamma}(G)$ and $\Gamma_{0\gamma}^*(G)$ into one physically irreducible irep $R_\gamma^{(1)}(G)$, the resulting $R_\gamma^{(1)}$-covariant is not unique; namely, if (x_γ, y_γ) is an $R_\gamma^{(1)}$-covariant, then so also is $(y_\gamma, -x_\gamma)$. We have already discussed this consequence of Schur lemma II in connection with the standard transformation from complex variables to real ones (Kopský 1976b). Of the two $R_\gamma^{(1)}$-covariants we give always only one.

The denominator invariants are distinguished by underlining. As shown in I, our derivation yields the minimal integrity basis. If the number of invariants exceeds d_α, then certainly there are numerator invariants. In all cases we get them easily by checking algebraic relations. Due to the simplicity we do not give the syzygies here.

With the use of these typical EIBs we calculated the EIBs for vector representations of the 32 ordinary point groups. These are given in table A2 of the Appendix. The choice of ireps of non-centrosymmetrical groups is related to the choice of the proper rotation group to which they are isomorphic, so that elements with the same rotational part are represented by the same matrices (compare with a standard choice of ireps for tensorial covariants (Kopský 1979a, b)). The Γ-labelling is correlated in table A2 with the usual spectroscopic notation of Heine (1960).

5. Examples

5.1. Irreducible matrix groups

Let us consider an irep. $R_3^{(1)}(x_3, y_3)$ of the group D_3; it is faithful, and polynomials in x_3, y_3 provide covariants to ireps $\Gamma_1(x_1)$ and $\Gamma_2(x_2)$ of D_3. The irep $R_5^{(1)}(x_5, y_5)$ of the group D_6 is defined by the same matrices as $R_3^{(1)}(x_3, y_3)$ of D_3, with the difference that the unit matrix I_2 represents now the unit element e and twofold rotation 2_z of D_6: ker $R_5^{(1)} = \{e, 2_z\}$. The factor group D_6/C_2 is accordingly isomorphic to D_3, and each matrix of $R_3^{(1)}$ corresponds to two elements of D_6. Analogously ker $R_5^{(1)+}(D_{6h}) = \{e, 2_z, i, m_z\}$, ker $R_3^{(1)}(O) = \{e, 2_x, 2_y, 2_z\} = D_2$ and ker $R_3^{(1)+}(O_h) = D_{2h}$, where all factor groups D_{6h}/C_{2h}, O/D_2, O_h/D_{2h} are isomorphic to D_3. All these ireps generate the identity irep itself and one one-dimensional irep of the group in question, and the EIBs for them are represented by the EIBs of $\mathscr{P}(x_3, y_3)$.

A useful example are the two ireps $\Gamma_4^{(1)-}(x_4^-, y_4^-, z_4^-)$ and $\Gamma_5^{(1)-}(x_5^-, y_5^-, z_5^-)$ of the group O_h. Both are faithful and consist of the same matrices, but the mapping of O_h onto the matrix group is different. From the CG table we have $(x_5^-, y_5^-, z_5^-) \approx x_2^+(x_4^-, y_4^-, z_4^-)$ and conversely $(x_4^-, y_4^-, z_4^-) \approx x_2^+(x_5^-, y_5^-, z_5^-)$. Since $(x_2^+)^2$ is an invariant, we see at once that even degrees of r_4^-, r_5^- form the same covariants of even parity, while odd degrees differ as if the covariants are multiplied by x_2^+. Investigating this situation closely we shall find that it is due to an outer automorphism of O_h which leaves invariant the subgroup T_h and exchanges the cosets (O–T) and i(O–T). In terms of typical variables, this automorphism leaves all even-parity variables unchanged and reshifts the odd-parity ones as shown in table A1.

One-dimensional ireps have a special position in this scheme. The kernel of a direct sum of these ireps is the derived group H of G (commutator group of G), and the factor group G/H is abelian. For the abelian group we are able to express the EIB in its typical form involving all variables. So, for example, the group D_4–$4_z 2_x 2_{xy}$ has derived group $C_2 = \{e, 2_z\}$ with factor group $D_4/C_2 = \{e, 2_z\} + \{4_z, 4_z^{-1}\} + \{2_x, 2_y\} + \{2_{xy}, 2_{x\bar{y}}\}$ isomorphic to D_2. The EIBs of all algebras which do not contain variables transforming as (x_5, y_5) can be found at once from the typical EIBs of the group D_2 (Kopský 1975):

$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3(x_3)$	$\Gamma_4(x_4)$
x_2^2 x_3^2 x_4^2 $x_2x_3x_4$	x_3x_4	x_2x_4	x_2x_3

5.2. Extended integrity basis of $\mathscr{P}(x_5, y_5)$ for the group D_4

Let us first reproduce the table of CG products for D_4:

$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3(x_3)$	$\Gamma_4(x_4)$	$R_5^{(1)}(x_5, y_5)$
x_2^2 x_3^2 x_4^2	x_3x_4	x_2x_4	x_2x_3	$x_2(y_5, -x_5)$
$x_5^2+y_5^2$	$x_5y_5-y_5x_5$	$x_5^2-y_5^2$	$x_5y_5+y_5x_5$	$x_3(x_5, -y_5)$
				$x_4(y_5, x_5)$

The steps of the algorithm are as follows: *1st degree.* Only the basic linear covariants $(x, y) \approx (x_5, y_5)$(further we drop indices 5). *2nd degree.* The CG table provides an invariant $I_0 = x^2+y^2$, Γ_3-covariant x^2-y^2 and Γ_4-covariant xy. *3rd degree.* We get one reducible $R_5^{(1)}$-covariant $\boldsymbol{a}_0 = I_0(x, y) = (x^3+xy^2, y^3+x^2y)$, and from CG products we obtain $R_5^{(1)}$-covariants $\boldsymbol{a}_1 = (x^2-y^2)(x, -y) = (x^3-xy^2, y^3-x^2y)$ and $\boldsymbol{a}_2 = xy(y, x) = (xy^2, x^2y)$. There is a linear relation $\boldsymbol{a}_1 + 2\boldsymbol{a}_2 = \boldsymbol{a}_0$ so that $\boldsymbol{a}_0$ is the basis of reducible covariants and one of $\boldsymbol{a}_1, \boldsymbol{a}_2$ suffices to complete the basis; we take $\boldsymbol{a}_1 + \boldsymbol{a}_2 = (x^3, y^3)$. *4th degree.* From (x^3, y^3) we get at once the irreducible invariant $I_1 = x^4+y^4$. The $\boldsymbol{a}_1, \boldsymbol{a}_2$ produce invariants $(x^2-y^2)^2$ and x^2y^2 which have the same relation with I_1, I_0^2 as $\boldsymbol{a}_1, \boldsymbol{a}_2$ have with $\boldsymbol{a}_1+\boldsymbol{a}_2, \boldsymbol{a}_0$. The Γ_2-covariant x^3y-y^3x is irreducible, and no other Γ_2-covariant is produced because the product of (x, y) with $\boldsymbol{a}_0$ vanishes. The Γ_3- and Γ_4-covariants $x^4-y^4 = I_0(x^2-y^2)$ and $x^3y+xy^3 = I_0xy$ are reducible, and again there are no others because $((xy^2, x^2y), (x, y))_3 = 0$, $((x^3-xy^2, y^3-x^2y), (x, y))_4 = 0$. *5th degree.* There remains only one irreducible Γ_2-covariant in the table which gives the $R_5^{(1)}$-covariant $(x^3y^2-xy^4, x^2y^3-x^4y)$. We find easily that this is a difference of reducible covariants $I_0(x^3, y^3)$ and $I_1(x, y)$, which, together with the third reducible covariant $I_0^2(x, y)$, form the full basis of 5th-degree $R_5^{(1)}$-covariants.

5.3. Extended integrity basis of vector representation of D_4

First we find by inspection that components of vector (x, y, z) transform under D_4 as $z \approx x_2$ and $(x, y) \approx (x_5, y_5)$. The EIB of $\mathscr{P}(x, y)$ is a copy of the EIB of $\mathscr{P}(x_5, y_5)$ and consists of denominator invariants x^2+y^2 and x^4+y^4, Γ_2-covariant $xy(x^2-y^2)$, Γ_3-covariant x^2-y^2, Γ_4-covariant xy, and two $R_5^{(1)}$-covariants (x, y) and (x^3, y^3). The EIB of $\mathscr{P}(z)$ is a copy of that of $\mathscr{P}(x_2)$ for the group C_2 (recall that $\ker \Gamma_2(D_4) = C_4$, $D_4/C_4 \approx C_2$) and consists of denominator invariant z^2 and Γ_2-covariant z. Multiplying $\mathscr{P}(x, y) \otimes \mathscr{P}(z)$ according to the table of CG products we get in addition a numerator invariant $xyz(x^2-y^2)$, Γ_3-covariant xyz, Γ_4-covariant $(x^2-y^2)z$, and two $R_5^{(1)}$-covariants $z(y, -x)$ and $z(y^3, -x^3)$. Except for the last $R_5^{(1)}$-covariant all of them are clearly irreducible. To check the irreducibility of $z(y^3, -x^3)$ we have to compare it with reducible covariants of the same overall homogeneous degree (1 in z and 3 in (x, y)). There is only one such covariant, namely $(x^2+y^2)(y, -x)z$, and $z(y^3, -x^3)$ is also irreducible.

6. Use of extended integrity bases in phase transition theory

In the usual Landau model of phase transitions one uses truncated thermodynamic potentials. Let us consider, for example, possible transitions from the group D_4 with the transition parameter belonging to the two-dimensional irep. One finds easily the macroscopic tensorial meaning of typical variables: $x_2 \approx P_z$, $x_3 \approx \Delta u = u_1 - u_2$, $x_3 \approx u_6$, and $(x_5, y_5) \approx (P_x, P_y) \approx (u_4, u_5)$, where $\boldsymbol{P}$ is the polarisation and $\boldsymbol{u}$ the deformation tensor. The symmetry D_4–$4_z2_x2_{xy}$ forbids non-zero polarisation and allows deformation components u_3 and $u_1 = u_2$. Let the transition parameter be the polarisation. Then we shall write the usual Landau (truncated polynomial) potential as

$$A_0(T-T_c)(P_x^2+P_y^2)+A_1(P_x^4+P_y^4)+A_2P_x^2P_y^2+\ldots+B_0P_z^2+B_1P_z^4+\ldots+C_0u_6^2$$
$$+C_1u_6^4+\ldots+D_0(\Delta u)^2+D_1(\Delta u)^4+\ldots+E_0(u_4^2+u_5^2)+E_1(u_4^4+u_5^4)$$
$$+E_2u_4^2u_5^2+\text{coupling terms.}$$

Using integrity bases we can write the potential compactly in the form

$$f_0(P_0, P_1)+f_1(P_z^2)+f_2(u_6^2)+f_3(\Delta u^2)+u_6P_xP_yg(P_0, P_1)$$
$$+\Delta u(P_x^2-P_y^2)h(P_0, P_1)+P_zP_xP_y(P_x^2-P_y^2)k(P_0, P_1)$$

where $P_0 = P_x^2+P_y^2$, $P_1 = P_x^4+P_y^4$, f_i, g, h, k are functions. This form is not quite a general invariant function, but it contains all coupling terms of primary importance, and function f_0 gives the most general invariant function of the transition parameter. One sees, for example, that solutions $P_x = 0$, $P_y = 0$ (transition into symmetry 2_y, 2_x respectively) lead to $u_6 = 0$, $P_z = 0$; solutions $P_x = P_y$, $P_x = -P_y$ (transitions into 2_{xy}, $2_{x\bar{y}}$ respectively) lead to $\Delta u = 0$, $P_z = 0$; while the general solution leads to non-zero values of these variables. These, of course, are conclusions which follow also from symmetry considerations without an analysis of the potential. But now we are not restricted to the use of the Landau singularity $A_0(T-T_c)P_0^2$; the function f_0 is also a function of T with a certain singularity at T_c, and this singularity can be varied. Such model potentials could be useful in modern 'renormalisation' theories in which, as far as we know, the symmetry arguments have not yet been used.

7. Conclusions

Extended integrity bases of irreducible matrix groups relevant to crystal point groups enable the construction of any such bases. The phenomenology of phase transitions provides one of the motivations for their use. The quantum mechanical motivations are considered by Patera *et al* (1978). The mathematical content of the results given is very exhaustive—we can now express functional invariants as well as covariants in any desired set of variables for the crystal and magnetic point groups.

Appendix

Table A1. Extended integrity bases of irreducible matrix groups—of crystal point groups.

$\Gamma_2(C_2)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$
	$\underline{x^2}$	

$R_3^{(1)}(C_3)$	$\Gamma_1(x_1)$	$R_3^{(1)}(x_3, y_3)$
	x^2+y^2	$(x^2-y^2; -2xy)$
	$\underline{x^3-3xy^2}$	
	$\underline{y^3-3x^2y}$	

$R_3^{(1)}(D_3)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$R_3^{(1)}(x_3, y_3)$
	$\underline{x^2+y^2}$		$(x^2-y^2; -2xy)$
	$\underline{x^3-3xy^2}$	y^3-3x^2y	

$R_5^{(1)}(C_4)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$R_5^{(1)}(x_5, y_5)$
	x^2+y^2	$x^2-y^2 \quad xy$	(x^3, y^3)
	$\underline{x^4+y^4}$		
	$\underline{xy(x^2-y^2)}$		

$\Gamma_3(C_3)$	$\Gamma_1(x_1)$	$\Gamma_3(\xi_3)$	$\Gamma_3^*(\eta_3)$
	$\xi\eta$	η^2	ξ^2
	$\underline{\xi^3} \quad \underline{\eta^3}$		

$\Gamma_3^{(1)}(D_3)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3^{(1)}(\xi_3, \eta_3)$
	$\underline{\xi\eta}$		(η^2, ξ^2)
	$\underline{\xi^3+\eta^3}$	$\xi^3-\eta^3$	

$\Gamma_5^{(1)}(C_4)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_5(\xi_5)$	$\Gamma_5^*(\eta_5)$
	$\xi\eta$	$\xi^2 \quad \eta^2$	η^3	ξ^3
	$\underline{\xi^4} \quad \underline{\eta^4}$			

$\Gamma_5^{(1)}(D_4)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3(x_3)$	$\Gamma_4(x_4)$	$\Gamma_5^{(1)}(\xi_5, \eta_5)$
	$\underline{\xi\eta}$		$\xi^2+\eta^2$	$\xi^2-\eta^2$	(η^3, ξ^3)
	$\underline{\xi^4+\eta^4}$	$\xi^4-\eta^4$			

Table A1. (continued)

$R_5^{(1)}(\mathrm{D}_4)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3(x_3)$	$\Gamma_4(x_4)$	$R_5^{(1)}(x_5, y_5)$
	$\underline{x^2+y^2}$		x^2-y^2	xy	(x^3, y^3)
	$\underline{x^4+y^4}$	$xy(x^2-y^2)$			

$\Gamma_6^{(1)}(\mathrm{C}_6)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_5(\xi_5)$	$\Gamma_5^*(\eta_5)$	$\Gamma_6(\xi_6)$	$\Gamma_6^*(\eta_6)$
	$\xi\eta$		η^2	ξ^2		
		$\xi^3 \quad \eta^3$				
			ξ^4	η^4		
					η^5	ξ^5
	$\underline{\xi^6} \quad \underline{\eta^6}$					

$R_6^{(1)}(\mathrm{C}_6)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$R_5^{(1)}(x_5, y_5)$	$R_6^{(1)}(x_6, y_6)$
	x^2+y^2		$(x^2-y^2, -2xy)$	
		x^3-3xy^2		
		$y-3x^2y$		
			$(x^4-6x^2y^2+y^4, 4xy(x^2-y^2))$	
				$(x^5-10x^3y^2+5xy^4, -y^5+10x^2y^3-5x^4y)$
	$\underline{x^6-15x^4y^2+15x^2y^4-y^6}$			
	$\underline{xy(x^2-3y^2)(y^2-3x^2)}$			

$\Gamma_6^{(1)}(\mathrm{D}_6)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3(x_3)$	$\Gamma_4(x_4)$	$\Gamma_5^{(1)}(\xi_5, \eta_5)$	$\Gamma_6^{(1)}(\xi_6, \eta_6)$
	$\underline{\xi\eta}$				(η^2, ξ^2)	
			$\xi^3+\eta^3$	$\xi^3-\eta^3$		
					(ξ^4, η^4)	
						(η^5, ξ^5)
	$\underline{\xi^6+\eta^6}$	$\xi^6-\eta^6$				

Table A1. (continued)

$R_6^{(1)}(D_6)$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$\Gamma_3(x_3)$	$\Gamma_4(x_4)$	$R_5^{(1)}(x_5, y_5)$	$R_6^{(1)}(x_6, y_6)$
	$\underline{x^2+y^2}$				$(x^2-y^2, -2xy)$	
			x^3-3xy^2	y^3-3x^2y		
					$(x^4-6x^2y^2+y^4, 4xy(x^2-y^2))$	
						$(x^5-10x^3y^2+5xy^4, -y^5+10x^2y^3-5x^4y)$
	$\underline{x^6-15x^4y^2+15x^2y^4-y^6}$	$(x^3-3xy^2)(y^3-3x^2y)$				

$\Gamma_4^{(1)}(T)$	$\Gamma_1(x_1)$	$R_3^{(1)}(x_3, y_3)$	$\Gamma_4^{(1)}(x_4, y_4, z_4)$
	$\underline{x^2+y^2+z^2}$	$(x^2-a(y^2+z^2), b(y^2-z^2))$	(yz, zx, xy)
	$\underline{xyz}$		(x^3, y^3, z^3)
			$(x(z^2-y^2), y(x^2-z^2), z(y^2-x^2))$
	$\underline{x^4+y^4+z^4}$	$(x^4-a(y^4+z^4), b(y^4-z^4))$	$(yz(z^2-y^2), zx(x^2-z^2), xy(y^2-x^2))$
			$(x(z^4-y^4), y(x^4-z^4), z(y^4-x^4))$
	$x^2(z^4-y^4)+y^2(x^4-z^4)+z^2(y^4-x^4)$		

$\Gamma_4^{(1)-}(T_h)$	$\Gamma_1^+(x_1^+)$	$R_3^{(1)+}(x_3^+, y_3^+)$	$\Gamma_4^{(1)+}(x_4^+, y_4^+, z_4^+)$
	$\underline{x^2+y^2+z^2}$	$(x^2-a(y^2+z^2), b(y^2-z^2))$	(yz, zx, xy)
	$\underline{x^4+y^4+z^4}$		$(yz(z^2-y^2), zx(x^2-z^2), xy(y^2-x^2))$
	$\underline{x^2y^2z^2}$		
	$x^2(z^4-y^4)+y^2(x^4-z^4)+z^2(y^4-x^4)$		

Even degree ≈ even parity.

Table A1. (continued)

$\Gamma_4^{(1)-}(\mathrm{T_h})$	$\Gamma_1^-(x_1^-)$	$R_3^{(1)-}(x_3^-, y_3^-)$	$\Gamma_4^{(1)-}(x_4^-, y_4^-, z_4^-)$
	xyz		(x^3, y^3, z^3)
			$(x(z^2-y^2), y(x^2-z^2), z(y^2-x^2))$
		$xyz(x^2-a(y^2+z^2), b(y^2-z^2))$	$xyz(yz, zx, xy)$
			$(x(z^4-y^4), y(x^4-z^4), z(y^4-x^4))$

Odd degree ≈ odd parity.

$\Gamma_4^{(1)}(\mathrm{O})$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$R_3^{(1)}(x_3, y_3)$	$\Gamma_4^{(1)}(x_4, y_4, z_4)$	$\Gamma_5^{(1)}(x_5, y_5, z_5)$
	$\underline{x^2+y^2+z^2}$		$(z^2-a(x^2+y^2), b(x^2-y^2))$	(yz, zx, xy)	
	$\underline{xyz}$			(x^3, y^3, z^3)	$(x(z^2-y^2), y(x^2-z^2), z(y^2-x^2))$
	$\underline{x^4+y^4+z^4}$		$(z^4-a(x^4+y^4), b(x^4-y^4))$		$(yz(z^2-y^2), zx(x^2-z^2), xy(y^2-z^2))$
					$(x(z^4-y^4), y(x^4-z^4), z(y^4-x^4))$
		$x^2(z^4-y^4)+y^2(x^4-z^4)+z^2(y^4-x^4)$			

$\Gamma_5^{(1)}(\mathrm{O})$	$\Gamma_1(x_1)$	$\Gamma_2(x_2)$	$R_3^{(1)}(x_3, y_3)$	$\Gamma_4^{(1)}(x_4, y_4, z_4)$	$\Gamma_5^{(1)}(x_5, y_5, z_5)$
	$\underline{x^2+y^2+z^2}$		$(z^2-a(x^2+y^2), b(x^2-y^2))$	(yz, zx, xy)	
		xyz		$(x(z^2-y^2), y(x^2-z^2), z(y^2-z^2))$	(x^3, y^3, z^3)
	$\underline{x^4+y^4+z^4}$		$(z^4-a(x^4+y^4), b(x^4-y^4))$	$xyz(x, y, z)$	$(yz(z^2-y^2), zx(x^2-z^2), xy(y^2-x^2))$
			$xyz(b(x^2-y^2), a(x^2+y^2)-z^2)$	$(x(z^4-y^4), y(x^4-z^4), z(y^4-x^4))$	$xyz(yz, zx, xy)$
	$\underline{(xyz)^2}$	$x^2(z^4-y^4)+y^2(x^4-z^4)$ $+z^2(y^4-x^4)$		$xyz(x^3, y^3, z^3)$	$xyz(x(z^2-y^2), y(x^2-z^2), z(y^2-x^2))$
			$xyz(b(x^4-y^4), a(x^4+y^4)-z^4)$	$xyz(yz(z^2-y^2), zx(x^2-z^2), xy(y^2-x^2))$	
					$xyz(x(z^4-y^4), y(x^4-z^4), z(y^4-x^4))$
	$xyz[x^2(z^4-y^4)+y^2(x^4-z^4)+z^2(y^4-x^4)]$				

Table A1. (continued)

$\Gamma_5^{(1)-}(O_h)$	$\Gamma_1^+(x_1^+)$	$\Gamma_2^+(x_2^+)$	$R_3^{(1)+}(x_3^+, y_3^+)$	$\Gamma_4^{(1)+}(x_4^+, y_4^+, z_4^+)$	$\Gamma_5^{(1)+}(x_5^+, y_5^+, z_5^+)$
$\Gamma_4^{(1)-}(O_h)$	$\Gamma_1^+(x_1^+)$	$\Gamma_2^+(x_2^+)$	$R_3^{(1)+}(x_3^+, y_3^+)$	$\Gamma_4^{(1)+}(x_4^+, y_4^+, z_4^+)$	$\Gamma_5^{(1)+}(x_5^+, y_5^+, z_5^+)$
	$\underline{x^2+y^2+z^2}$ $\underline{x^4+y^4+z^4}$ $\underline{(xyz)^2}$	$x^2(z^4-y^4)+y^2(x^4-z^4)+z^2(y^4-x^4)$	$(z^2-a(x^2+y^2), b(x^2-y^2))$ $(z^4-a(x^4+y^4), b(x^4-y^4))$	(yz, zx, xy) $xyz(x, y, z)$ $xyz(x^3, y^3, z^3)$	$(yz(z^2-y^2), zx(x^2-z^2), xy(y^2-x^2))$ $xyz(x(z^2-y^2), y(x^2-z^2), z(y^2-x^2))$ $xyz(x(z^4-y^4), y(x^4-z^4), z(y^4-x^4))$

Even degree ≈ even parity.

$\Gamma_5^{(1)-}(O_h)$	$\Gamma_1^-(x_1^-)$	$\Gamma_2^-(x_2^-)$	$R_3^{(1)-}(x_3^-, y_3^-)$	$\Gamma_4^{(1)-}(x_4^-, y_4^-, z_4^-)$	$\Gamma_5^{(1)-}(x_5^-, y_5^-, z_5^-)$
$\Gamma_4^{(1)-}(O_h)$	$\Gamma_2^-(x_1^-)$	$\Gamma_1^-(x_1^-)$	$R_3^{(2)-}(y_3^-, -x_3^-)$	$\Gamma_5^{(1)-}(x_5^-, y_5^-, z_5^-)$	$\Gamma_4^{(1)-}(x_4^-, y_4^-, z_4^-)$
	$xyz[x^2(z^4-y^4)+y^2(x^4-z^4)+z^2(y^4-x^4)]$	xyz	$xyz(b(x^2-y^2), a(x^2+y^2)-z^2)$ $xyz(b(x^4-y^4), a(x^4+y^4)-z^4)$	$(x(z^2-y^2), y(x^2-z^2), z(y^2-x^2))$ $(x(z^4-y^4), y(x^4-z^4), z(y^4-x^4))$ $xyz(yz(z^2-y^2), zx(x^2-z^2), xy(y^2-x^2))$	(x^3, y^3, z^3) $xyz(yz, zx, xy)$

Odd degree ≈ odd parity. $a = 1/2$, $b = \sqrt{3}/2$ in all cubic groups.

Table A2. Extended integrity bases of polynomial algebras on vector representations of crystal point groups.

Triclinic, monoclinic and orthorhombic groups

C_1–1: trivial; A–$\Gamma_1(x_1)$: $\underline{x}, \underline{y}, \underline{z}$.

C_i–$\bar{1}$: A_g–$\Gamma_1^+(x_1^+)$: $\underline{x^2}, \underline{y^2}, \underline{z^2}, xy, yz, zx$; A_u–$\Gamma_1^-(x_1^-)$: x, y, z.

C_2–2_z: A–$\Gamma_1(x_1)$: $\underline{z}, \underline{x^2}, \underline{y^2}, xy$; B–$\Gamma_2(x_2)$: x, y.

C_s–m_z: A′–$\Gamma_1(x_1)$: $\underline{x}, \underline{y}, \underline{z^2}$; A″–$\Gamma_2(x_2)$: z.

C_{2h}–$2_z/m_z$: A_g–$\Gamma_1^+(x_1^+)$: $\underline{x^2}, \underline{y^2}, \underline{z^2}, xy$; B_g–$\Gamma_2^+(x_2^+)$: xz, yz; A_u–$\Gamma_1^-(x_1^-)$: z; B_u–$\Gamma_2^-(x_2^-)$: x, y.

D_2–$2_x2_y2_z$: A–$\Gamma_1(x_1)$: $\underline{x^2}, \underline{y^2}, \underline{z^2}, xyz$; B_1–$\Gamma_2(x_2)$: z, xy; B_3–$\Gamma_3(x_3)$: x, yz; B_2–$\Gamma_4(x_4)$: y, zx.

C_{2v}–$m_xm_y2_z$: A_1–$\Gamma_1(x_1)$: $\underline{z}, \underline{x^2}, \underline{y^2}$; A_2–$\Gamma_2(x_2)$: xy; B_2–$\Gamma_3(x_3)$: y; B_1–$\Gamma_4(x_4)$: x.

D_{2h}–$m_xm_ym_z$: A_g–$\Gamma_1^+(x_1^+)$: $\underline{x^2}, \underline{y^2}, \underline{z^2}$; B_{1g}–$\Gamma_2^+(x_2^+)$: xy; B_{3g}–$\Gamma_3^+(x_3^+)$: yz; B_{2g}–$\Gamma_4^+(x_4^+)$: zx; A_u–$\Gamma_1^-(x_1^-)$: xyz; B_{1u}–$\Gamma_2^-(x_2^-)$: z; B_{3u}–$\Gamma_3^-(x_3^-)$: x; B_{2u}–$\Gamma_4^-(x_4^-)$: y.

Tetragonal groups

C_4–4_z: A–$\Gamma_1(x_1)$: $\underline{z}, \underline{x^2+y^2}, \underline{x^4+y^4}, \underline{xy(x^2-y^2)}$; B–$\Gamma_2(x_2)$: xy, x^2-y^2;
E–$R_5^{(1)}(x_5, y_5)$: $(x, y), (x^3, y^3)$.

S_4–$\bar{4}_z$: A–$\Gamma_1(x_1)$: $x^2+y^2, \underline{z^2}, xyz, (x^2-y^2)z, \underline{x^4+y^4}, \underline{xy(x^2-y^2)}$; B–$\Gamma_2(x_2)$: z, xy, x^2-y^2;
E–$R_5^{(1)}(x_5, y_5)$: $(y, x), z(x, y), (y^3, x^3)$.

C_{4h}–$4_z/m_z$: A_g–$\Gamma_1^+(x_1^+)$: $x^2+y^2, \underline{z^2}, \underline{x^4+y^4}, \underline{xy(x^2-y^2)}$; B_g–$\Gamma_2^+(x_2^+)$: xy, x^2-y^2;
E_g–$R_5^{(1)+}(x_5^+, y_5^+)$: $z(x, y), z(x^3, y^3)$; A_u–$\Gamma_1^-(x_1^-)$: z; B_u–$\Gamma_2^-(x_2^-)$: $xyz, (x^2-y^2)z$;
E_u–$R_5^{(1)-}(x_5^-, y_5^-)$: $(x, y), (x^3, y^3)$.

D_4–$4_z2_x2_{xy}$: A_1–$\Gamma_1(x_1)$: $\underline{x^2+y^2}, \underline{z^2}, \underline{x^4+y^4}, xyz(x^2-y^2)$; A_2–$\Gamma_2(x_2)$: $z, xy(x^2-y^2)$;
B_1–$\Gamma_3(x_3)$: x^2-y^2, xyz; B_2–$\Gamma_4(x_4)$: $xy, (x^2-y^2)z$;
E–$R_5^{(1)}(x_5, y_5)$: $(x, y), z(y, -x), (x^3, y^3), z(y^3, -x^3)$.

C_{4v}–$4_zm_xm_{xy}$: A_1–$\Gamma_1(x_1)$: $\underline{z}, \underline{x^2+y^2}, \underline{x^4+y^4}$; A_2–$\Gamma_2(x_2)$: $xy(x^2-y^2)$; B_1–$\Gamma_3(x_3)$: x^2-y^2; B_2–$\Gamma_4(x_4)$: xy;
E–$R_5^{(1)}(x_5, y_5)$: $(y, -x), (y^3, -x^3)$.

D_{2d}–$\bar{4}_z2_xm_{xy}$: A_1–$\Gamma_1(x_1)$: $\underline{x^2+y^2}, \underline{z^2}, xyz, \underline{x^4+y^4}$; A_2–$\Gamma_2(x_2)$: $(x^2-y^2)z, xy(x^2-y^2)$; B_1–$\Gamma_3(x_3)$: x^2-y^2;
B_2–$\Gamma_4(x_4)$: z, xy; E–$R_5^{(1)}(x_5, y_5)$: $(x, -y), z(y, -x), (x^3, -y^3)$.

D_{2d}–$\bar{4}_zm_x2_{xy}$: A_1–$\Gamma_1(x_1)$: $\underline{x^2+y^2}, \underline{z^2}, (x^2-y^2)z, \underline{x^4+y^4}$; A_2–$\Gamma_2(x_2)$: $xyz, xy(x^2-y^2)$; B_2–$\Gamma_3(x_3)$: z, x^2-y^2;
B_1–$\Gamma_4(x_4)$: xy; E–$R_5^{(1)}(x_5, y_5)$: $(y, x), z(y, -x), (y^3, x^3)$.

D_{4h}–$4_z/m_zm_xm_{xy}$: A_{1g}–$\Gamma_1^+(x_1^+)$: $\underline{x^2+y^2}, \underline{z^2}, \underline{x^4+y^4}$; A_{2g}–$\Gamma_2^+(x_2^+)$: $xy(x^2-y^2)$; B_{1g}–$\Gamma_3^+(x_3^+)$: x^2-y^2;
B_{2g}–$\Gamma_4^+(x_4^+)$: xy; E_g–$R_5^{(1)+}(x_5^+, y_5^+)$: $z(y, -x), z(y^3, -x^3)$; A_{1u}–$\Gamma_1^-(x_1^-)$: $xyz(x^2-y^2)$; A_{2u}–$\Gamma_2^-(x_2^-)$: z;
B_{1u}–$\Gamma_3^-(x_3^-)$: xyz; B_{2u}–$\Gamma_4^-(x_4^-)$: $(x^2-y^2)z$; E_u–$R_5^{(1)-}(x_5^-, y_5^-)$: $(x, y), (x^3, y^3)$.

Table A2. (continued)

Trigonal and hexagonal groups

C_3–3_z: A–$\Gamma_1(x_1)$: z, x^2+y^2, $x(x^2-3y^2)$, $y(y^2-3x^2)$; E–$R_3^{(1)}(x_3, y_3)$: (x, y), $(x^2-y^2;\ -2xy)$.

S_6–$\bar{3}_z$: A_g–$\Gamma_1^+(x_1^+)$: x^2+y^2, z^2, $xz(x^2-3y^2)$, $yz(y^2-3x^2)$, $xy(x^2-3y^2)(y^2-3x^2)$, $x^6-15x^4y^2+15x^2y^4-y^6$; E_g–$R_3^{(1)+}(x_3^+, y_3^+)$: $z(x, y)$, $(x^2-y^2;\ -2xy)$, $(x^4-6x^2y^2+y^4;\ 4xy(x^2-y^2))$; A_u–$\Gamma_1^-(x_1^-)$: z, $x(x^2-3y^2)$, $y(y^2-3x^2)$; E_u–$R_3^{(1)-}(x_3^-, y_3^-)$: (x, y), $z(x^2-y^2;\ -2xy)$, $(x^5-10x^3y^2+5xy^4;\ -y^5+10x^2y^3-5x^4y)$.

D_3–3_z2_x: A_1–$\Gamma(x_1)$: x^2+y^2, z^2, $x(x^2-3y^2)$, $yz(y^2-3x^2)$; A_2–$\Gamma_2(x_2)$: z, $y(y^2-3x^2)$; E–$R_3^{(1)}(x_3, y_3)$: (x, y), $z(y, -x)$, $(x^2-y^2;\ -2xy)$, $z(2xy;\ x^2-y^2)$.

C_{3v}–3_zm_x: A_1–$\Gamma_1(x_1)$: z, x^2+y^2, $y(y^2-3x^2)$; A_2–$\Gamma_2(x_2)$: $x(x^2-3y^2)$; E–$R_3^{(1)}(x_3, y_3)$: $(y, -x)$, $(x^2-y^2;\ -2xy)$.

D_{3d}–$\bar{3}_zm_x$: A_{1g}–$\Gamma_1^+(x_1^+)$: x^2+y^2, z^2, $yz(y^2-3x^2)$, $x^6-15x^4y^2+15x^2y^4-y^6$; A_{2g}–$\Gamma_2^+(x_2^+)$: $xz(x^2-3y^2)$, $xy(x^2-3y^2)(y^2-3x^2)$; E_g–$R_3^{(1)+}(x_3^+, y_3^+)$: $z(y, -x)$, $(x^2-y^2;\ -2xy)$, $(x^4-6x^2y^2+y^4;\ 4xy(x^2-y^2))$, $z(y^5-10x^2y^3+5x^4y;\ x^5-10x^3y^2+5xy^4)$; A_{1u}–$\Gamma_1^-(x_1^-)$: $x(x^2-3y^2)$, $xyz(x^2-3y^2)(y^2-3x^2)$; A_{2u}–$\Gamma_2^-(x_2^-)$: z, $y(y^2-3x^2)$; E_u–$R_3^{(1)-}(x_3^-, y_3^-)$: (x, y), $z(2xy;\ x^2-y^2)$, $(x^5-10x^3y^2+5xy^4;\ -y^5+10x^2y^3-5x^4y)$.

C_6–6_z: A–$\Gamma_1(x_1)$: z, x^2+y^2, $x^6-15x^4y^2+15x^2y^4-y^6$, $xy(x^2-3y^2)(y^2-3x^2)$; B–$\Gamma_2(x_2)$: $x(x^2-3y^2)$, $y(y^2-3x^2)$; E_2–$R_5^{(1)}(x_5, y_5)$: $(x^2-y^2;\ -2xy)$, $(x^4-6x^2y^2+y^4;\ 4xy(x^2-y^2))$; E_1–$R_6^{(1)}(x_6, y_6)$: (x, y), $(x^5-10x^3y^2+5xy^4;\ -y^5+10x^2y^3-5x^4y)$.

C_{3h}–$\bar{6}_z$: A′–$\Gamma_1(x_1)$: x^2+y^2, z^2, $x(x^2-3y^2)$, $y(y^2-3x^2)$; A″–$\Gamma_2(x_2)$: z; E′–$R_5^{(1)}(x_5, y_5)$: (x, y), $(x^2-y^2;\ -2xy)$; E″–$R_6^{(1)}(x_6, y_6)$: $z(x, y)$, $z(x^2-y^2;\ -2xy)$.

C_{6h}–$6_z/m_z$: A_g–$\Gamma_1^+(x_1^+)$: x^2+y^2, z^2, $x^6-15x^4y^2+15x^2y^4-y^6$, $xy(x^2-3y^2)(y^2-3x^2)$; B_g–$\Gamma_2^+(x_2^+)$: $xz(x^2-3y^2)$, $(yz(y^2-3x^2))$; E_{2g}–$R_5^{(1)+}(x_5, y_5)$: $(x^2-y^2;\ -2xy)$, $(x^4-6x^2y^2+y^4;\ 4xy(x^2-y^2))$;
E_{1g}–$R_6^{(1)+}(x_6^+, y_6^+)$: $z(x, y)$, $z(x^5-10x^3y^2+5xy^4;\ -y^5+10x^2y^3-5x^4y)$; A_u–$\Gamma_1^-(x_1^-)$: z; B_u–$\Gamma_2^-(x_2^-)$: $x(x^2-3y^2)$, $y(y^2-3x^2)$; E_{2u}–$R_5^{(1)-}(x_5^-, y_5^-)$: $z(x^2-y^2;\ -2xy)$, $z(x^4-6x^2y^2+y^4;\ 4xy(x^2-y^2))$; E_{1u}–$R_6^{(1)-}(x_6^-, y_6^-)$: (x, y), $(x^5-10x^3y^2+5xy^4;\ -y^5+10x^2y^3-5x^4y)$.

D_6–$6_z2_x2_y$: A_1–$\Gamma_1(x_1)$: x^2+y^2, z^2, $x^6-15x^4y^2+15x^2y^4-y^6$, $xyz(x^2-3y^2)(y^2-3x^2)$; A_2–$\Gamma_2(x_2)$: z, $xy(x^2-3y^2)(y^2-3x^2)$; B_2–$\Gamma_3(x_3)$: $x(x^2-3y^2)$, $yz(x^2-3y^2)$; B_1–$\Gamma_4(x_4)$: $y(y^2-3x^2)$, $xz(x^2-3y^2)$; E_2–$R_5^{(1)}(x_5, y_5)$: $(x^2-y^2;\ -2xy)$, $z(2xy;\ x^2-y^2)$, $(x^4-6x^2y^2+y^4;\ 4xy(x^2-y^2))$, $z(4xy(y^2-x^2);\ x^4-6x^2y^2+y^4)$; E_1–$R_6^{(1)}(x_6, y_6)$: (x, y), $z(y, -x)$, $(x^5-10x^3y^2+5xy^4;\ -y^5+10x^2y^3-5x^4y)$, $z(y^5-10x^2y^3+5x^4y;\ x^5-10x^3y^2+5xy^4)$.

C_{6v}–$6_zm_xm_y$: A_1–$\Gamma_1(x_1)$: z, x^2+y^2, $x^6-15x^4y^2+15x^2y^4-y^6$; A_2–$\Gamma_2(x_2)$: $xy(x^2-3y^2)(y^2-3x^2)$; B_1–$\Gamma_3(x_3)$: $y(y^2-3x^2)$; B_2–$\Gamma_4(x_4)$: $x(x^2-3y^2)$; E_2–$R_5^{(1)}(x_5, y_5)$: $(x^2-y^2;\ -2xy)$, $(x^4-6x^2y^2+y^4;\ 4xy(x^2-y^2))$; E_1–$R_6^{(1)}(x_6, y_6)$: $(y, -x)$, $(y^5-10x^2y^3+5x^4y;\ x^5-10x^3y^2+5xy^4)$.

D_{3h}–$\bar{6}_z2_xm_y$: A_1'–$\Gamma_1(x_1)$: x^2+y^2, z^2, $x(x^2-3y^2)$; A_2'–$\Gamma_2(x_2)$: $y(y^2-3x^2)$; A_1''–$\Gamma_3(x_3)$: $yz(y^2-3x^2)$; A_2''–$\Gamma_4(x_4)$: z; E′–$R_5^{(1)}(x_5, y_5)$: (x, y), $(x^2-y^2;\ -2xy)$; E″–$R_6^{(1)}(x_6, y_6,)$: $z(y, -x)$, $z(2xy, x^2-y^2)$.

D_{3h}–$\bar{6}_zm_x2_y$: A_1'–$\Gamma_1(x_1)$: x^2+y^2, z^2, $y(y^2-3x^2)$; A_2'–$\Gamma_2(x_2)$: $x(x^2-3y^2)$; A_2''–$\Gamma_3(x_3)$: z; A_1''–$\Gamma_4(x_4)$: $xz(x^2-3y^2)$; E′–$R_5^{(1)}(x_5, y_5)$: $(y, -x)$, $(x^2-y^2;\ -2xy)$; E″–$R_6^{(1)}(x_6, y_6)$: $z(y, -x)$, $z(x^2-y^2;\ -2xy)$.

Table A2. (continued)

Trigonal and hexagonal groups (continued)

$\mathrm{D_{6h}}$–$6_z/\mathrm{m}_z\mathrm{m}_x\mathrm{m}_y$: $\mathrm{A_{1g}}$–$\Gamma_1^+(x_1^+)$: $\underline{x^2+y^2}$, $\underline{z^2}$, $\underline{x^6-15x^4y^2+15x^2y^4-y^6}$;
$\mathrm{A_{2g}}$–$\Gamma_2^+(x_2^+)$: $xy(x^2-3y^2)(y^2-3x^2)$; $\mathrm{B_{2g}}$–$\Gamma_3^+(x_3^+)$: $yz(y^2-3x^2)$;
$\mathrm{B_{1g}}$–$\Gamma_4^+(x_4^+)$: $xz(x^2-3y^2)$; $\mathrm{E_{2g}}$–$R_5^{(1)+}(x_5^+, y_5^+)$: $(x^2-y^2;\ -2xy)$, $(x^4-6x^2y^2+y^4;\ 4xy(x^2-y^2))$;
$\mathrm{E_{1g}}$–$R_6^{(1)+}(x_6^+, y_6^+)$: $z(y, -x)$, $z(y^5-10x^2y^3+5x^4y;\ x^5-10x^3y^2+5xy^4)$;
$\mathrm{A_{1u}}$–$\Gamma_1^-(x_1^-)$: $xyz(x^2-3y^2)(y^2-3x^2)$; $\mathrm{A_{2u}}$–$\Gamma_2^-(x_2^-)$: z; $\mathrm{B_{2u}}$–$\Gamma_3^-(x_3^-)$: $x(x^2-3y^2)$;
$\mathrm{B_{1u}}$–$\Gamma_4^-(x_4^-)$: $y(y^2-3x^2)$; $\mathrm{E_{2u}}$–$R_5^{(1)-}(x_5^-, y_5^-)$: $z(2xy;\ x^2-y^2)$, $z(4xy(y^2-x^2);\ x^4-6x^2y^2+y^4)$;
$\mathrm{E_{1u}}$–$R_6^{(1)-}(x_6^-, y_6^-)$: (x, y), $(x^5-10x^3y^2+5xy^4;\ -y^5+10x^2y^3-5x^4y)$.

Cubic groups

Vector representation of each cubic group is identical with one of its ireps, and hence the EIBs are contained in table A1. The correspondence of vector representation in spectroscopic notation to our Γ-notation is as follows: T–$\Gamma_4(x_4, y_4, z_4)$ and $\mathrm{T_u}$–$\Gamma_4^-(x_4^-, y_4^-, z_4^-)$ in groups T and $\mathrm{T_h}$; $\mathrm{T_1}$–$\Gamma_5(x_5, y_5, z_5)$ and $\mathrm{T_{1u}}$–$\Gamma_5^-(x_5^-, y_5^-, z_5^-)$ in groups O and $\mathrm{O_h}$; and $\mathrm{T_2}$–$\Gamma_4(x_4, y_4, z_4)$ in group $\mathrm{T_d}$ under the convention that elements of $\mathrm{T_d}$ with the same proper rotational parts are represented by the same matrices as those of O.

Warning. The extended integrity bases given are the minimal ones and do not contain all numerator invariants.

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