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Complete Reduction Bases for the Principal Induced Representations of the Crystallographic Point Groups

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Abstract

An ordered partition P of a point group G is constructed in left cosets $H_{\dots\beta\alpha} = \dots B^{\beta}A^{\alpha}H$ related to a subgroup H by means of selected genitors $A, B, \dots$:

$$P = \{H_{\dots\beta\alpha} \mid \alpha = 1 \text{ to } a, \beta = 1 \text{ to } b, \dots\},$$

$$ab\dots = |G|/|H|.$$

This partition P spans a principal induced representation (PIR) $R(H:G)$ of G. Then a basis L of this PIR is built:

$$L = \{V_{\dots kj} \mid j = 1 \text{ to } a, k = 1 \text{ to } b, \dots\}$$

with

$$V_{\dots kj} = \dots \sum_{\beta=1}^{b} \sum_{\alpha=1}^{a} \exp[2i\pi(\dots + k\beta/b + j\alpha/a)]H_{\dots\beta\alpha}.$$

In many cases L is a complete reduction basis (CRB) of $R(H:G)$ for which all matrices are fully reduced. The possibility of obtaining such a CRB depends on the algebraic structure of the group G, on the considered subgroup H and on the choice of genitors $A, B, \dots$. Methods are proposed using subgroup chain properties, invariant inductor subgroup properties, direct product properties etc. These methods have been applied to crystallographic point groups. Complete tables of CRBs are recorded for all PIRs of all crystallographic point groups except for a few PIRs of the point groups 432, $\bar{4}3m$ and $m\bar{3}m$.

Introduction

In practice the reduction of a reducible representation Γ of a group is not an easy task. The purpose is not only to determine the irreducible representations (IR) which are the components of Γ but also to find a basis of the representation vector space for which the matrices of Γ are all in a reduced form. When each irreducible component appears once only, the projection operators are usually used (Schonland, 1971; Bradley & Cracknell, 1972; Labarre, 1978); they lead to the required basis by a more or less laborious task. 'The problem is more complicated when the same IR appears several times in Γ.... There is no general method... one proceeds as best as one can, guiding oneself according to the form of the matrices of Γ' (Schonland, 1971).* In the case of induced representations, reduction methods have been proposed by Bradley & Cracknell (1972) which applied to representations induced by invariant subgroups.

In the present paper we will show that it is often possible in the case of a principal induced representation (PIR) of a point group G, to build a reduced basis; it is not necessary to use the group algebra $\mathscr{A}$ of G but a vector subspace Ω, the dimension of which is smaller than that of $\mathscr{A}$;† the vectors of this subspace are the cosets of the partition of G relating to the subgroup H inducing the PIR of G. It is not necessary for H to be invariant in G; no matrix diagonalization is needed in the reduction process; only the knowledge of the group multiplication table is required. An application of the method is to be able to propose basis vectors and reduced matrices for each IR of G.

I. Building the ordered partition

The PIR properties of a group are well known (Lomont, 1959; Murnagham, 1963; Kirillov, 1976).

* After the French edition.

† Except in the event of an inductor subgroup reduced to the identity element. In this case Ω is identical to $\mathscr{A}$.

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Litvin (1982), Berenson, Kotzev & Litvin (1982), Litvin, Kotzev & Birman (1982), Masmoudi & Billiet (1989) have given numerous applications to crystallography.

Consider a point group G of order $|G|$ and the left partition P of G relating to a subgroup H of order $|H|$ distinct from G. We construct P as follows. Consider an element A of G not contained in H and designate the left coset $A^\alpha H$ by H_α. Form the set P_A of different cosets H_α:

$$P_A=\{H_1, H_2, H_3, \ldots, H_a\}=\{H_\alpha \mid \alpha=1,2,3,\ldots,a\}.$$

The number a is called the degree of the genitor A, a is such that $\alpha>a$ involves the formation of cosets already found.* Note that a is not necessarily the order of A but divides it. A must be chosen in such a manner that a divides the index p of H in G $(p=|G|/|H|)$. If $P_A\neq P$, choose another element B of G not contained in any coset of P_A and form the set P_B of cosets $H_{\beta\alpha}$, with $H_{\beta\alpha}=B^\beta H_\alpha=B^\beta A^\alpha H$:

$$P_B=\{H_{\beta\alpha} \mid \alpha=1,2,\ldots,a;\ \beta=1,2,\ldots,b\}.$$

The degree b of the genitor B is such that $\beta>b$ involves the formation of cosets already found in P_B. b divides the order of B. B must be chosen in such a manner that b is greater than 1 and divides p/a.† Note that it is often useful to take the element B as a first genitor if A is a power of B. If $P_B\neq P$, the process is repeated to obtain the full left partition P of G related to H:

$$P=\{H_{\ldots\gamma\beta\alpha}=\ldots C^\gamma B^\beta A^\alpha H \mid \alpha=1 \text{ to } a,\ \beta=1 \text{ to } b,\ \gamma=1 \text{ to } c,\ldots\}.$$

One says that the partition P is ordered by labels $H_{\ldots\gamma\beta\alpha}$. The degrees $a, b, c, \ldots$ of the genitors‡ $A, B, C, \ldots$ fulfil the condition $abc\ldots=p$. In most cases, there are several ways to order P because several choices are possible for the first genitor, then for the second one, and so on.§ Finally, in the trivial case $H=G$, one may consider that a unique genitor is needed, it is of course included in H and its degree is 1.

* That is to say, A^a is the lowest power of A contained in H.

† The fact that B is not contained in P_A does not involve $b>1$. *Example*: $G=432$, $H=3_{a+b+c}2_{\substack{-a+b\\ -b+c\\ a-c}}$, $A=2^1_{a+b}$, $a=2$, $B=2^1_{a+c}$ and $b=1$!

‡ The elements $A, B, C, \ldots$ are called the genitors of the ordered partition to avoid any confusion with the generators of a group (or a subgroup), the meaning of which is entirely different.

§ But in every way of ordering P, the subgroup H is always the last coset to appear: $H=H_{\ldots cba}$. Note that if one changes the appearance order of the elements used as genitors, the required partition does not necessarily result; for $G=432$, $H=3_{a+b+c}2_{\substack{-a+b\\ -b+c\\ a-c}}$, an ordered partition with $A=2^1_{a+b}$, $B=2^1_a$ results but one constructs no partition of G relating to H with $A=2^1_a$ and $B=2^1_{a+b}$!

Table 1. *Group $G=32$, subgroup $H=1$, four genitor choices for P*

The first column gives the choice number. The second and third columns give the chosen genitors. The following six columns refer to the labels $H_{\alpha\beta}$ of the different cosets of the partition. In the present case ($H=1$), each coset is composed of a single element.

No.	A	B	(2^1_b)	(2^1_{-a-b})	(2^1_a)	(3^1)	(3^2)	(1^1)
1	3^1	2^1_a	H^1_{11}	H^1_{12}	H^1_{13}	H^1_{21}	H^1_{22}	H^1_{23}
2	3^2	2^1_a	H^2_{12}	H^2_{11}	H^2_{13}	H^2_{22}	H^2_{21}	H^2_{23}
3	3^1	2^1_b	H^3_{13}	H^3_{11}	H^3_{12}	H^3_{21}	H^3_{22}	H^3_{23}
4	2^1_a	3^1	H^4_{21}	H^4_{11}	H^4_{31}	H^4_{12}	H^4_{22}	H^4_{32}

Example 1

$$G=\bar{4}_c 2_{\substack{a\\ b}} m_{\substack{a+b\\ -a+b}},\ |G|=8,\ H=2_c=\{2^1_c, 1^1\},\ |H|=2,$$

$A=\bar{4}^1$, $a=2$, $B=2^1_a$, $b=2$, $ab=4=p$.

$$P_A=\{\bar{4}^1.H, 2^1_c.H\}=\{(\bar{4}^3, \bar{4}^1), (1^1, 2^1_c)\}=\{H_1, H_2\},$$

$$P_B=\{2^1_a.\bar{4}^1.H, 2^1_a.2^1_c.H, \bar{4}^1.H, 2^1_c.H\}$$
$$=\{(m^1_{a+b}, m^1_{-a+b}), (2^1_a, 2^1_b), (\bar{4}^3, \bar{4}^1), (1^1, 2^1_c)\}^*$$
$$=\{H_{11}, H_{12}, H_{21}, H_{22}\}=P.$$

There are 23 other ways to order P because six choices are possible for A ($\bar{4}^1, \bar{4}^3, 2^1_a, 2^1_b, m^1_{a+b}, m^1_{-a+b}$), then four choices are possible for B in the event of $A=\bar{4}^1$ (*i.e.* $2^1_a, 2^1_b, m^1_{a+b}, m^1_{-a+b}$) and so on.

Example 2

$$G=3_c 2_{\substack{a\\ b\\ -a-b}},\ |G|=6,\ H=1=\{1^1\},\ |H|=1,\ A=3^1,$$

$a=3$, $B=2^1_a$, $b=2$, $ab=6=p$.

$$P_A=\{3^1.H, 3^2.H, 1^1.H\}=\{(3^1), (3^2), (1^1)\}$$
$$=\{H_1, H_2, H_3\},$$
$$P_B=\{2^1_a.3^1.H, 2^1_a.3^2.H, 2^1_a.H, 3^1.H, 3^2.H, 1^1.H\}$$
$$=\{(2^1_b), (2^1_{-a-b}), (2^1_a), (3^1), (3^2), (1^1)\}$$
$$=\{H_{11}, H_{12}, H_{13}, H_{21}, H_{22}, H_{23}\}=P.$$

There exist altogether 12 ways to order P depending on the choice of genitors. Some are recorded in Table 1.

II. Building the basis related to the ordered partition

To simplify the writing, we suppose that two genitors are sufficient to order the partition P but the theoretical account remains true in principle whatever the

* The chronological order of symmetry-operation products goes from right to left: the meaning of $X.Y$ is X preceded by Y.

actual number of genitors may be. It is known that the p partition cosets are a basis of the vector space Ω over the field $\mathbb{C}$ of the PIR $R(H:G)$ of G relating to H. Unfortunately, this basis does not lead to reduced matrices. We construct a new basis of Ω related to the ordered partition, it allows reduced matrices to be obtained on numerous occasions and thus basis vectors for each IR constituting $R(H:G)$. First it is necessary to define a scalar product in Ω as follows: $(H_s . H_t) = (1/p)\delta_{st}$ with H_s and H_t any two cosets of P; therefore the p vectors $p^{1/2}H_s$ are unit orthogonal vectors, they constitute a basis of Ω and any vector of Ω is expressed by $V = \sum_{s=1}^{p} x_s H_s$ with $x_s \in \mathbb{C}$. The value of the scalar product of two vectors of Ω is given by $(V. V') = (1/p)\sum_{s=1}^{p} x_s x_s'^*$ ($x_s'^*$: complex conjugate of x_s').

For any representation (reducible or not) of a group, it is well known that a basis may be chosen for which the matrix of any element of G is unitary: its eigenvalues are some rth complex roots of 1, r being the order of the represented element. Then construct the following p vectors ($1 \le k \le b, 1 \le j \le a$):

$$V_{kj} = \sum_{\beta=1}^{b} \sum_{\alpha=1}^{a} \exp[2i\pi(k\beta/b + j\alpha/a)] H_{\beta\alpha}.$$

These p vectors are unit orthogonal and constitute a basis L of Ω because

$$(V_{kj} . V_{k'j'}) = (1/p) \sum_{\beta} \exp[2i\pi(k-k')\beta/b] \times \sum_{\alpha} \exp[2i\pi(j-j')\alpha/a] = \delta_{kk'}\delta_{jj'}.$$

Note that each vector V_{kj} is an eigenvector for the genitor B and its powers because one has: $B . V_{kj} = \exp(-2i\pi k/b) V_{kj}$. Thus the matrices of the PIR $R(H:G)$ are fully diagonalized for the elements B^n in the basis L. The action on a given vector V_{kj} of other elements X of G leads, by means of a projection on the basis L of the transformed vectors $X . V_{kj}$, to determine a subspace of Ω containing V_{kj}: this subspace is invariant by G. In practice, it is sufficient to consider only the action of generators of G belonging to distinct conjugation classes. Therefore V_{kj} and the vectors of L which transform together with V_{kj} under the action of such generators form a basis of a subrepresentation of $R(H:G)$. More often than not this subrepresentation is irreducible and it is easy to identify its Mulliken notation by means of its trace values using character tables. The last vector of L, namely V_{ba}, always generates the identical representation (contained in any PIR). If all so-obtained subrepresentations are irreducible, the matrices of $R(H:G)$ are entirely reduced in the basis L. Then this basis is called a complete reduction basis (CRB) of the considered PIR. The case $H = G$ is trivial: $R(H:G)$ clearly is the identical representation, the basis of which is the vector $V = G$.

Table 2. *Characters of the IRs of group* $\bar{4}2m$

	1^1	$2.\bar{4}^1$	2_c^1	2.2_a^1	$2.m_{a+b}^1$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	−1	1	1	−1
B_2	1	−1	1	−1	1
E	2	0	−2	0	0

Example 1 (*continued*)

$G = \bar{4}2m$, $H = 2_c$, $A = \bar{4}^1$, $a = 2$, $B = 2_a^1$, $b = 2$. Generators of G: $\bar{4}^1$, 2_a^1.

$$V_{11} = H_{11} - H_{12} - H_{21} + H_{22} = (m_{a+b}^1, m_{-a+b}^1) - (2_a^1, 2_b^1) - (\bar{4}^3, \bar{4}^1) + (1^1, 2_c^1),$$

$$V_{12} = -H_{11} - H_{12} + H_{21} + H_{22},$$

$$V_{21} = -H_{11} + H_{12} - H_{21} + H_{22},$$

$$V_{22} = H_{11} + H_{12} + H_{21} + H_{22}.$$

$$\bar{4}^1 . V_{11} = (2_b^1, 2_a^1) - (m_{a+b}^1, m_{-a+b}^1) - (1^1, 2_c^1) + (\bar{4}^1, \bar{4}^3) = H_{12} - H_{11} - H_{22} + H_{21} = -V_{11}, \quad \chi = -1,$$

$$\bar{4}^1 . V_{12} = -H_{12} - H_{11} + H_{22} + H_{21} = V_{12}, \quad \chi = 1,$$

$$\bar{4}^1 . V_{21} = -H_{12} + H_{11} - H_{22} + H_{21} = -V_{21}, \quad \chi = -1,$$

$$\bar{4}^1 . V_{22} = H_{12} + H_{11} + H_{22} + H_{21} = V_{22}, \quad \chi = 1,$$

$$2_a^1 . V_{11} = \exp(-2i\pi/2) V_{11} = -V_{11}, \quad \chi = -1,$$

$$2_a^1 . V_{12} = \exp(-2i\pi/2) V_{12} = -V_{12}, \quad \chi = -1,$$

$$2_a^1 . V_{21} = \exp(-2i\pi . 2/2) V_{21} = V_{21}, \quad \chi = 1,$$

$$2_a^1 . V_{22} = \exp(-2i\pi . 2/2) V_{22} = V_{22}, \quad \chi = 1.$$

The vector V_{11} transforms alone and generates the IR B_2 because $\chi(\bar{4}^1) = -1$ and $\chi(2_a^1) = -1$ (*cf.* Table 2). In the same way, V_{12} generates A_2, V_{21} generates B_1 and V_{22} generates A_1.

To conclude: $R(2_c : \bar{4}2m) = B_2 + A_2 + B_1 + A_1$. In the basis $L = [V_{11}, V_{12}, V_{21}, V_{22}]$ built in this way, the matrices of the PIR are fully reduced.

III. Influence of the choice of genitors and of the group structure complexity

When the structure of the group G is not too complex (cyclic groups and their direct and semi-direct products), there always exists at least a choice of genitors enabling a CRB to be found whatever the considered PIR, *i.e.* whatever the subgroup H.

Table 3. *Characters of the IRs of group* 4

	1^1	4^1	2^1	4^3
A	1	1	1	1
B	1	−1	1	1
E (1)	1	i	−1	$-i$
E (2)	1	$-i$	−1	i

Example 3

$G=4$. Generator: 4^1.

(a) $H=2=\{2^1, 1^1\}$, $A=4^1$, $a=2$.

$$P_A=\{(4^3,4^1),(1^1,2^1)\}=\{H_1,H_2\}=P.$$

$$V_1=-H_1+H_2,\quad V_2=H_1+H_2,$$

$$4^1 . V_1=-V_1,\quad 4^1 . V_2=V_2.$$

V_1 generates the IR B and V_2 generates the IR A of 4 (*cf.* Table 3): $[V_1, V_2]$ is indeed a CRB of $R(2:4)=B+A$.

(b) $H=1=\{1^1\}$, $A=4^3$, $a=4$.

$$P_A=\{(4^3),(2^1),(4^1),(1^1)\}$$
$$=\{H_1,H_2,H_3,H_4\}=P,$$
$$V_1=iH_1-H_2-iH_3+H_4,$$
$$V_2=-H_1+H_2-H_3+H_4$$
$$V_3=iH_1-H_2+iH_3+H_4,$$
$$V_4=H_1+H_2+H_3+H_4.$$
$$4^1 . V_1=iV_1,\quad 4^1 . V_2=-V_2,$$
$$4^1 . V_3=-iV_3,\quad 4^1 . V_4=V_4.$$

V_1 generates the complex IR $E(1)$ (*cf.* Table 3), V_3 generates the complex conjugate IR $E(2)$, V_2 is a basis for the IR B and V_4 is a basis for the IR A. $[V_1, V_2, V_3, V_4]$ is of course a CRB of $R(1:4)=E(1)+E(2)+B+A$.

Example 2 (*continued*)

$G=32$, $H=1$. The 12 ways of ordering P all lead to a CRB. We are going to compare the CRBs relating to the four genitor choices of Table 1. 3^1 and 2^1_a are the generators of G.

(a) *Choice* 1. Here is the basis L^1 [$j=\exp(2i\pi/3)$]:

$$V^1_{11}=-jH^1_{11}-j^2H^1_{12}-H^1_{13}+jH^1_{21}+j^2H^1_{22}+H^1_{23},$$
$$V^1_{12}=-j^2H^1_{11}-jH^1_{12}-H^1_{13}+j^2H^1_{21}+jH^1_{22}+H^1_{23},$$
$$V^1_{13}=-H^1_{11}-H^1_{12}-H^1_{13}+H^1_{21}+H^1_{22}+H^1_{23},$$
$$V^1_{21}=jH^1_{11}+j^2H^1_{12}+H^1_{13}+jH^1_{21}+j^2H^1_{22}+H^1_{23},$$
$$V^1_{22}=j^2H^1_{11}+jH^1_{12}+H^1_{13}+j^2H^1_{21}+jH^1_{22}+H^1_{23},$$
$$V^1_{23}=H^1_{11}+H^1_{12}+H^1_{13}+H^1_{21}+H^1_{22}+H^1_{23}.$$

Let us call W the transformed vector of V^1_{11} by the generator 3^1:

$$W=3^1 . V^1_{11}$$
$$=-jH^1_{13}-j^2H^1_{11}-H^1_{12}+jH^1_{22}+j^2H^1_{23}+H^1_{21}.$$

Table 4. *Characters of the IRs of the group* $\bar{3}2/m$

The first three rows and the first three columns give the characters of the IRs of the group 32 (delete the subscript g of the Mulliken notation).

	1^1	2.3^1	3.2^1_a	$\bar{1}^1$	$2.\bar{3}^1$	$3.m^1_a$
A_{1g}	1	1	1	1	1	1
A_{2g}	1	1	−1	1	1	−1
E_g	2	−1	0	2	−1	0
A_{1u}	1	1	1	−1	−1	−1
A_{2u}	1	1	−1	−1	−1	1
E_u	2	−1	0	−2	1	0

To determine the components of W, we are projecting it on L^1 using the scalar products (*cf.* § II).

$$(W . V^1_{11})=\tfrac{1}{6}(-j . -1-j^2 . -j^2-1 . -j$$
$$+j . j+j^2 . 1+1 . j^2)=-\tfrac{1}{2},$$
$$(W . V^1_{12})=0,\quad (W . V^1_{13})=0,$$
$$(W . V^1_{21})=-i3^{1/2}/2,$$
$$(W . V^1_{22})=0,\quad (W, V^1_{23})=0.$$

Then we have: $W=3^1 . V^1_{11}=-\frac{1}{2}V^1_{11}-(i3^{1/2}/2)V^1_{21}$. In the same way we obtain: $3^1 . V^1_{12}=-\frac{1}{2}V^1_{12}+(i3^{1/2}/2)V^1_{22}$, $3^1 . V^1_{13}=V^1_{13}$, $3^1 . V^1_{21}=-(i3^{1/2}/2)V^1_{11}-\frac{1}{2}V^1_{21}$, $3^1 . V^1_{22}=(i3^{1/2}/2)V^1_{12}-\frac{1}{2}V^1_{22}$, $3^1 . V^1_{23}=V^1_{23}$, $2^1_a . V^1_{11}=-V^1_{11}$, $2^1_a . V^1_{12}=-V^1_{12}$, $2^1_a . V^1_{13}=-V^1_{13}$, $2^1_a . V^1_{21}=V^1_{21}$, $2^1_a . V^1_{22}=V^1_{22}$, $2^1_a . V^1_{23}=V^1_{23}$.

So V^1_{11} and V^1_{21} are transformed together and are a basis for an IR of type E (compare the traces of 3^1 and 2^1_a with the characters given in Table 4). Likewise V^1_{12} and V^1_{22} are transformed together and are a basis for another IR of the same type E, V^1_{13} spans the IR A_2 and V^1_{23} generates the IR A_1. Therefore L^1 is a CRB for $R(1:32)=2E+A_2+A_1$.

(b) *Choice* 2. In an analogous manner, the basis L^2 is constructed and its transformed vectors are projected on L^2. One finds: $(V^2_{11}, V^2_{21}):E$, $(V^2_{12}, V^2_{22}):E$, $V^2_{13}:A_2$, $V^2_{23}:A_1$. Now let us project the vectors of L^2 on L^1. It follows that $V^2_{11}=V^1_{12}$, $V^2_{21}=V^1_{22}$, so that (V^2_{11}, V^2_{21}) spans the same IR of type E as (V^1_{12}, V^1_{22}). Likewise (V^2_{12}, V^2_{22}) and (V^1_{11}, V^1_{21}) span the other IR of type E because $V^2_{12}=V^1_{11}$ and $V^2_{22}=V^1_{21}$. In the same way, $V^2_{13}=V^1_{13}:A_2$ and $V^2_{23}=V^1_{23}:A_1$.

(c) *Choice* 3. One proceeds likewise for L^3. (V^3_{11}, V^3_{21}) spans the same type E IR as (V^1_{11}, V^1_{21}) because

$$V^3_{11}=-(j/2)V^1_{11}+[(3+i3^{1/2})/4]V^1_{21},$$
$$V^3_{21}=[(3+i3^{1/2})/4]V^1_{11}-(j/2)V^1_{21};$$

(V^3_{12}, V^3_{22}) and (V^1_{12}, V^1_{22}) span the other type E IR because

$$V^3_{12} = -(j^2/2)V^1_{12} + [(3 - i3^{1/2})/4]V^1_{22},$$
$$V^3_{22} = [(3 - i3^{1/2})/4]V^1_{12} - (j^2/2)V^1_{22};$$
$$V^3_{13} = V^1_{13}: A_2,\ V^3_{23} = V^1_{23}: A_1.$$

It would be false to conclude that the four invariant subspaces E, E, A_2, A_1 exhibited by any genitor choice do not depend on the considered choice! In fact:

(*d*) *Choice* 4. In the former three choices, the genitor A belongs to the conjugation class of 3^1 in 32 and the genitor B belongs to the class of 2^1_a. In choice 4, the rôles are inverted. Here are the vectors of L^4:

$$V^4_{11} = -jH^4_{11} + jH^4_{12} - j^2H^4_{21} + j^2H^4_{22} - H^4_{31} + H^4_{32},$$
$$V^4_{12} = jH^4_{11} + jH^4_{12} + j^2H^4_{21} + j^2H^4_{22} + H^4_{31} + H^4_{32},$$
$$V^4_{21} = -j^2H^4_{11} + j^2H^4_{12} - jH^4_{21} + jH^4_{22} - H^4_{31} + H^4_{32},$$
$$V^4_{22} = j^2H^4_{11} + j^2H^4_{12} + jH^4_{21} + jH^4_{22} + H^4_{31} + H^4_{32},$$
$$V^4_{31} = -H^4_{11} + H^4_{12} - H^4_{21} + H^4_{22} - H^4_{31} + H^4_{32},$$
$$V^4_{32} = H^4_{11} + H^4_{12} + H^4_{21} + H^4_{22} + H^4_{31} + H^4_{32}.$$

After a projection of the transformed vectors on L^4, one gets: $3^1 . V^4_{11} = j^2V^4_{11}$, $3^1 . V^4_{12} = j^2V^4_{12}$, $3^1 . V^4_{21} = jV^4_{21}$, $3^1 . V^4_{22} = jV^4_{22}$, $3^1 . V^4_{31} = V^4_{31}$, $3^1 . V^4_{32} = V^4_{32}$, $2^1_a . V^4_{11} = -V^4_{21}$, $2^1_a . V^4_{12} = V^4_{22}$, $2^1_a . V^4_{21} = -V^4_{11}$, $2^1_a . V^4_{22} = V^4_{12}$, $2^1_a . V^4_{31} = -V^4_{31}$, $2^1_a . V^4_{32} = V^4_{32}$. This results in: $(V^4_{11}, V^4_{21}): E$, $(V^4_{12}, V^4_{22}): E$, $V^4_{31}: A_2$, $V^4_{32}: A_1$.

Let us now project the vectors of L^4 on L^1:

$$V^4_{11} = (V^1_{11} + V^1_{12} + V^1_{21} - V^1_{22})/2,$$
$$V^4_{12} = (V^1_{11} - V^1_{12} + V^1_{21} + V^1_{22})/2,$$
$$V^4_{21} = (V^1_{11} + V^1_{12} - V^1_{21} + V^1_{22})/2,$$
$$V^4_{22} = (-V^1_{11} + V^1_{12} + V^1_{21} + V^1_{22})/2,$$
$$V^4_{31} = V^1_{13},\ V^4_{32} = V^1_{23}.$$

The invariant one-dimensional subspaces A_1 and A_2 do not depend on the choice of genitors of the ordered partition. On the other hand, the two invariant two-dimensional subspaces of type E depend on the choice of genitors. In fact, one must consider that the four-dimensional subspace of the two IRs of type E forms a well defined whole which may be dissociated into two invariant subspaces in several distinct ways.

This surprising property of the algebra $\mathscr{A}$ of a non-Abelian group (*i.e.* a group possessing many-dimensional IRs) is not indicated in the classical treatises of group representation theory that we know, but it enlightens particularly the remark of Schonland (1971) quoted in the *Introduction.*

When the algebraic structure of the group G is complex, it is not always possible to find a choice of genitors which allows a CRB for those PIRs relating to subgroups of high index, and the obtained reduction is partial. Afterwards it is possible to resort to projection operators but we note that one then starts from a representation of which the dimension is much lower than that of the initial PIR.

Example 4

$G = 432$, $H = 2_{-a+b}$. The best reduction may be obtained using the following genitors: $A = 2^1_{a+b}$, $a = 2$, $B = 2^1_a$, $b = 2$, $C = 3^1_{a+b+c}$, $c = 3$. The next partial reduction is gained:*

$$(V_{111}, V_{121}, V_{211}, V_{221}, V_{311}, V_{321}): T_1 + T_2,$$
$$(V_{112}, V_{212}, V_{312}): T_2,\quad (V_{122}, V_{222}): E,\quad V_{322}: A_1.$$

The representation $T_1 + T_2$ may be reduced by means of projection operators.

The component T_1 receives the three vectors W_1, W_2, W_3 as a basis:

$$W_1 = H_{111} - H_{112} + H_{211} - H_{212} + H_{311} - H_{312},$$
$$W_2 = H_{121} - H_{122} - H_{221} + H_{222} + H_{311} - H_{312},$$
$$W_3 = H_{111} - H_{112} + H_{221} - H_{222} - H_{321} + H_{322}.$$

The three vectors W_4, W_5, W_6 constitute a basis for the component T_2:

$$W_4 = -H_{121} + H_{122} - H_{221} + H_{222} - H_{321} + H_{322},$$
$$W_5 = H_{121} - H_{122} + H_{211} - H_{212} - H_{311} + H_{312},$$
$$W_6 = -H_{111} + H_{112} + H_{221} - H_{222} + H_{311} - H_{312}.$$

Finally, if G_1, G_2 are two isomorphic groups and H_1, H_2 are respectively two isomorphic subgroups of them, then a CRB of $R(H_2: G_2)$ may be easily deduced from a CRB of $R(H_1: G_1)$; only the Mulliken notations may be changed.

Example 5

(*a*) $G_1 = 2/m$, $H_1 = \bar{1} = \{\bar{1}^1, 1^1\}$, $A_1 = 2^1$, $a_1 = 2$.

$$P = \{(m^1, 2^1), (\bar{1}^1, 1^1)\} = \{H_1, H_2\}.$$
$$V^1_1 = -H_1 + H_2,\quad V^1_2 = H_1 + H_2;$$
$$2^1 . V^1_1 = -V^1_1,\quad 2^1, V^1_2 = V^1_2,\quad \bar{1}^1 . V^1_1 = V^1_1,$$
$$\bar{1}^1 . V^1_2 = V^1_2;\quad V^1_1: B_g,\quad V^1_2: A_g\ (cf.\ \text{Table 5}).$$

(*b*) $G_2 = 222$, $H_2 = 2_a = \{2^1_a, 1^1\}$, $A_2 = 2^1_c$. It is sufficient to replace in the previous formulas the elements of $2/m$ by the corresponding elements of 222 to give: $V^2_1: B_3$, $V^2_2: A$ (*cf.* Table 5).

* For group character tables not given in the present paper, see for instance Atkins, Child & Phillips (1970).

Table 5. *Correspondence between the elements and the IRs of the groups 2/m and 222*

Characters of their IRs. The first two rows and the first two columns give the characters of the IRs of group 2 (delete the subscripts 3 and g of the Mulliken notation).

222		1^1	2^1_c	2^1_a	2^1_b
	$2/m$	1^1	2^1	$\bar{1}^1$	m^1
A	A_g	1	1	1	1
B_3	B_g	1	−1	1	−1
B_1	A_u	1	1	−1	−1
B_2	B_u	1	−1	−1	1

IV. The subgroup chain CRBs

Consider now two subgroups H and K of G such as $G \supset K \supset H$. It is known that the PIR of G relating to K is equivalent to a subrepresentation of the PIR of G relating to H, this is indicated as $R(K:G) \subset R(H:G)$ (Masmoudi & Billiet, 1989). It is also known that the PIRs relating to two conjugate subgroups H_1 and H_2 are equivalent, this is indicated as $R(H_1:G) = R(H_2:G)$. Let us see how these facts are expressed at the level of the CRBs.

Example 6

$G = 32.$

(*a*) $H_1 = 2_a = \{2^1_a, 1^1\}$, $A = 3^1$, $a = 3 = p$.

$$P^1 = \{(2^1_{-a-b}, 3^1), (2^1_b, 3^2), (2^1_a, 1^1)\}$$
$$= \{H^1_1, H^1_2, H^1_3\},$$
$$V^1_1 = jH^1_1 + j^2H^1_2 + H^1_3 = V^4_{12}$$

(*cf.* Example 2 continued and Table 1),

$$V^1_2 = j^2H^1_1 + jH^1_2 + H^1_3 = V^4_{22},$$
$$V^1_3 = H^1_1 + H^1_2 + H^1_3 = V^4_{32}.$$

Then: $(V^1_1, V^1_2):E$, $V^1_3:A_1$; $R(2_a:32) \subset R(1:32)$. In fact it would be false to conclude that the CRB of a PIR $R(H:32)$ constituted automatically of some vectors of the CRB L^4 of $R(1:32)$ whatever the subgroup H may be! For:

(*b*) $H_2 = 2_b = \{2^1_b, 1^1\}$, $A = 3^1$, $a = 3 = p$.

$$P^2 = \{(2^1_a, 3^1), (2^1_{-a-b}, 3^2), (2^1_b, 1^1)\}$$
$$= \{H^2_1, H^2_2, H^2_3\}.$$
$$V^2_1 = jH^2_1 + j^2H^2_2 + H^2_3,$$
$$V^2_2 = j^2H^2_1 + jH^2_2 + H^2_3,$$
$$V^2_3 = H^2_1 + H^2_2 + H^2_3.$$
$$3^1 \,.\, V^2_1 = j^2V^2_1, \quad 3^1 \,.\, V^2_2 = jV^2_2, \quad 3^1 \,.\, V^2_3 = V^2_3,$$
$$2^1_a \,.\, V^2_1 = jV^2_2, \quad 2^1_a \,.\, V^2_2 = j^2V^2_1, \quad 2^1_a \,.\, V^2_3 = V^2_3.$$
$$(V^2_1, V^2_2):E,\ V^2_3:A_1 \,.\, R(2_b:32) = R(2_a:32).$$

Now project these vectors on the bases L^1 and L^4 of $R(1:32)$:

$$V^2_1 = (V^1_{11} - jV^1_{12} + V^1_{21} + V^1_{22})/2$$
$$= [(3 - i3^{1/2})/4]V^4_{11} - (j^2/2)V^4_{12},$$
$$V^2_2 = (-j^2V^1_{11} + V^1_{12} + V^1_{21} + V^1_{22})/2$$
$$= [(3 + i3^{1/2})/4]V^4_{21} - (j/2)V^4_{22},$$
$$V^2_3 = V^1_{23} = V^4_{32}.$$

The CRBs of the PIRs $R(2_a:32)$ and $R(2_b:32)$ are different at the level of the irreducible component E, although these PIRs are equivalent and although the chosen genitor is the same in both cases. Moreover, the invariant subspace E of $R(2_b:32)$ is not confused with any of the four invariant subspaces of type E exhibited for $R(1:32)$! The reason that the vectors of the CRB of $R(2_a:32)$ belong to the CRB L^4 of $R(1:32)$ is the following. The first genitor used to construct L^4 is $A = 2^1_a$, thus one obtains $P_A = 2_a$, *i.e.* the partition of 2_a relating to 1. The second genitor is $B = 3^1$, *i.e.* the genitor used to construct the partition of 32 relating to 2_a.

One deduces from this example a process which constructs little by little the basis relating to a subgroup H_q end of the subgroup chain: $G \supset H_1 \supset H_2 \supset \cdots \supset H_q$.* Firstly, one tries to construct a CRB L_1 of $R(H_1:G)$. Then one tries to construct a CRB L_2 of $R(H_2:G)$ containing the vectors of L_1 by means of a partition of H_1 relating to H_2 for each coset of the partition of G relating to H_1; the same process is applied for the following subgroups of the chain to build $L_q: L_q \supset L_{q-1} \supset \cdots \supset L_2 \supset L_1$. Note that in this process the first genitor(s) of the partition of G relating to H_q is (are) the last found, the last genitor(s) is (are) found in the first step.

Example 7

$$G = 432, \quad H_1 = 4_a 2_{\substack{b\\c}} 2_{\substack{b+c\\-b+c}}, \quad H_2 = 4_a, \quad H_3 = 2_a.$$

$R(H_1:G)$ is constructed taking 3^1_{a+b+c} as a unique genitor, thus the CRB $L_1 = [V_1, V_2, V_3]$ is obtained: $(V_1, V_2):E$, $V_3:A_1$. Then $R(H_2:G)$ is constructed taking 2^1_b as a first genitor which enables one to find H_1 again, thus the CRB

$$L_2 = [V_{11}, V_{12} = V_1, V_{21}, V_{22} = V_2, V_{31}, V_{32} = V_3]$$

is obtained: $(V_{11}, V_{21}, V_{31}):T_1$, $(V_{12}, V_{22}):E$, $V_{32}:A_1$. Then $R(H_3:G)$ is constructed taking 4^1_a as a first genitor, which enables one to find H_2 again, thus the CRB L_3 is gained: $L_3 = [V_{111}, V_{112} = V_{11}, V_{121}, V_{122} = V_{12}, V_{211}, V_{212} = V_{21}, V_{221}, V_{222} = V_{22}, V_{311}, V_{312} = V_{31}, V_{321}, V_{322} = V_{32}]:(V_{111}, V_{211}, V_{311}):T_2, (V_{112}, V_{212}, V_{312}):T_1, (V_{121}, V_{221}):E, (V_{122}, V_{222}):E, V_{321}:A_2, V_{322}:A_1$. The genitors of $R(H_3:G)$ are $A = 4^1_a$, $B = 2^1_b$, $C = 3^1_{a+b+c}$.

* The process is of no interest if G is cyclic.

V. The case of an invariant inductor subgroup

When H is an invariant subgroup of G, let us call K a group isomorphic to the factor group G/H. Then the genitors of $R(H:G)$ are in a one-to-one correspondence with the genitors of $R(1:H)$, $R(H:G)$ and $R(1:H)$ are isomorphic. If there exists a CRB of $R(1:H)$ then there corresponds to it a CRB of $R(H:G)$. If K is an Abelian group, all IRs contained in $R(H:G)$ are one-dimensional. All this applies in the particular event where G is the semi-direct product $H\times K$ (this event occurs most frequenctly in crystallography),* then the genitors of $R(H:G)$ are confused with those of $R(1:H)$, only the Mulliken notations change.

Example 8
$G=\bar{3}2/m=H\times K$, $H=3$, $K=2_a/m_a\simeq G/H$. The genitors are $A=\bar{1}^1$ and $B=2_a^1$. This results in

$$R(1:2_a/m_a)=B_u+B_g+A_u+A_g,$$

$$R(3:\bar{3}2/m)=A_{2u}+A_{2g}+A_{1u}+A_{1g}$$

(*cf.* Tables 4 and 5).

If one goes over all cyclic subgroups K of G such there exists an invariant subgroup H of G with $G=H\times K$, then the PIR $R(H:G)$ provides all one-dimensional IRs of G. In particular, if $a=1$ ($H=G$), the identical IR is obtained. If $a=2$, in addition to the identical IR, an alternative IR is obtained, it is symmetrical with respect to the elements X of H and antisymmetrical with respect to the elements AX.

Example 9
$G=\bar{3}2/m=H\times K$, $H=\bar{3}$, $K=2_a\simeq G/H$, $A=2_a^1$,

$$R(\bar{3}:\bar{3}2/m)=A_{2g}+A_{1g}$$

$$\simeq R(1:2_a)=B+A \text{ (\textit{cf.} Table 5).}$$

If $a=3$, in addition to the identical IR, two complex conjugate IRs are obtained, they are symmetrical with respect to $X\in H$, their traces are respectively equal to $\exp(\pm 2i\pi/3)$ and $\exp(\pm 4i\pi/3)$ for the elements AX and A^2X.

Example 10
$G=\bar{3}=H\times K$, $H=\bar{1}$, $K=3\simeq G/H$, $A=3^1$.

$$R(\bar{1}:\bar{3})=E_g(2)+E_g(1)+A_g$$

$$\simeq R(1:3)=E(2)+E(1)+A.$$

If $a=4$, K contains $\{1^1, A^2\}$. Then, in addition to the identical IR and the alternative IR, $R(H:G)$ contains two complex conjugate IRs, they are symmetrical with respect to X and AX^2, their traces are equal to $\pm i$ and $\mp i$ for the elements AX and AX^3.

Example 11
$G=4/m=H\times K$, $H=m$, $K=4\simeq G/H$, $A=4^1$.

$$R(m:4/m)=E_u(2)+B_g+E_u(1)+A_g$$

$$\simeq R(1:4)=E(2)+B+E(1)+A.$$

If $a=6$, $R(H:G)$ contains the identical IR, an alternative IR and two pairs of complex conjugate IRs.

Example 12
$G=6/m=H\times K$, $H=2$, $K=\bar{3}\simeq G/H$, $A=\bar{3}^1$.

$$R(2:6/m)=E_{2u}(1)+E_{2g}(2)+A_u$$

$$+E_{2g}(1)+E_{2u}(2)+A_g$$

$$\simeq R(1:\bar{3})=E_u(1)+E_g(2)+A_u+E_g(1)+E_u(2)+A_g.$$

Finally, in the event of $G=H\times K$ with K a non-Abelian subgroup, $R(H:G)$ necessarily contains many-dimensional IRs.

Example 13
$G=\bar{3}2/m=H\times K$, $H=\bar{1}$, $K=32\simeq G/H$, $A=3^1$, $B=2_a^1$.

$$R(\bar{1}:\bar{3}2/m)=2E_g+A_{2g}+A_{1g}$$

$$\simeq R(1:32)=2E+A_2+A_1 \text{ (\textit{cf.} Table 2).}$$

VI. The direct product CRB

Now suppose that the group G is the direct product of a subgroup G_1 and a subgroup G_2; we consider here only the case where the order of G_2 is equal to 2 ($G_2=\{Y, 1^1\}$); this covers all cases met in crystallography; however, this process extends to groups G_2 of higher order. Suppose a CRB of $R(H_1:G_1)$ is known. Then it is easy to get a CRB of $R(H_1:G)$ and a CRB of $R(H:G)$, with H the direct product of H_1 and G_2.*

(1) Starting from the genitors† of the CRB L_1 of $R(H_1:G_1)$, the genitor Y is added to obtain the CRB L of $R(H_1:G)$. To each vector V_{kj} of L_1 correspond two vectors of L, *i.e.* $V_{1kj}=-Y.V_{kj}+V_{kj}=(-Y+1^1).V_{kj}$ and $V_{2kj}=(Y+1^1).V_{kj}$. To get a generator system of G, it is sufficient to add the element Y to the generators of G_1. Any generator X of G_1 transforms V_{1kj} and V_{2kj} just as V_{kj} because $X.V_{1kj}=X.(-Y+1^1).V_{kj}=(-Y+1^1).X.V_{kj}$ and $X.V_{2kj}=(Y+1^1).X.V_{kj}$ (remember that X commutes with Y

* Let us point out two cases for which G is not necessarily the semi-direct product of H by another subgroup. 1st case: $G=4$, $H=2$, $G/H\simeq H$ [*cf.* Example 3(*a*)] 2nd case: $G=D_3^*$, $H=R$, $D_3^*/R\simeq D_3=32$ (D_3 is not a subgroup of D_3^*) (see deposit).

* The process is of no interest if H_1 and H are invariant subgroups (see § V).

† We suppose here that two genitors are used to construct the CRB L_1; the process remains true whatever the genitor number may be.

and 1^1). On the other hand, Y transforms V_{1kj} into its opposite and keeps V_{2kj} invariant as $Y^2 = 1^1$. In other words, to each IR of $R(H_1:G_1)$ correspond two IRs of $R(H_1:G)$, the former is antisymmetrical with respect to Y [vector(s) V_{1kj}], the latter is symmetrical [vector(s) V_{2kj}].

Example 14

$G = \bar{3}2/m$, $G_1 = 32$, $G_2 = \bar{1}$, $H_1 = 2_a$. From Example 6(*a*), one gets the six vectors of the CRB of $R(2_a:\bar{3}2/m)$ (*cf.* Table 4):

$$V_{11} = -\bar{1}^1 \,.\, V_1^1 + V_1^1, \quad V_{12} = -\bar{1}^1 \,.\, V_2^1 + V_2^1,$$
$$V_{13} = -\bar{1}^1 \,.\, V_3^1 + V_3^1, \quad V_{21} = \bar{1}^1 \,.\, V_1^1 + V_1^1,$$
$$V_{22} = \bar{1}^1 \,.\, V_2^1 + V_2^1, \quad V_{23} = \bar{1}^1 \,.\, V_3^1 + V_3^1.$$
$$(V_{11}, V_{12}): E_u, \; V_{13}: A_{1u},$$
$$(V_{21}, V_{22}): E_g, \; V_{23}: A_{1g}.$$

(2) When $H = H_1 \otimes G_2$, one uses the fact that G/G_2 and H/G_2 are respectively isomorphic to G_1 and H_1. The CRB L of $R(H:G)$ is composed by as many vectors as the CRB L^1 of $R(H_1:G_1)$, their genitors are the same and each vector of L is obtained from the corresponding vector of L^1 replacing H_1 by H. The generators of G_1 transform the vectors of L in the same way as the vectors of L^1. The extra generator Y keeps invariant each vector of L. To each IR of $R(H_1:G_1)$ corresponds one IR of $R(H:G)$, it is symmetrical with respect to Y and it is also confused with the symmetrical IR previously met [*cf.* (1), vector(s) V_{2kj}].

Example 14 (*continued*)

$H = 2_a/m_a = H_1 \otimes G_2$. One gets immediately the three vectors of the CRB of $R(2_a/m_a:\bar{3}2/m)$ (*cf.* Table 4): $V_1 = V_{21}$, $V_2 = V_{22}$, $V_3 = V_{23}$; $(V_1, V_2): E_g$, $V_3: A_{1g}$.

VII. Results

Except for the case of groups 432, $\bar{4}3m$ and $4/m\,\bar{3}2/m$ to which we shall return, it has been possible for us to obtain CRBs for *all* PIRs of *all* crystallographic point groups using the processes proposed above. Starting from the CRBs of the PIRs of the groups $\bar{1}$, 4, 3, one obtains by means of an isomorphy those of the groups 2, m, $\bar{4}$, then by means of a direct product those of the groups $2/m$, 222, $mm2$, $4/m$, $\bar{3}$, 6, $\bar{6}$, $6/m$. Starting from the CRBs of 422, one gets by means of an isomorphy the CRBs of $4mm$, $\bar{4}2m$, then by means of direct products those of $4/m\;2/m\;2/m = 422 \otimes \bar{1} = 4mm \otimes \bar{1} = \bar{4}2m \otimes \bar{1}$. The same process is used starting from 32 to obtain the CRBs of $3m$, $\bar{3}2/m = 32 \otimes \bar{1} = 3m \otimes \bar{1}$; next one gets those of 622, $6mm$, $\bar{6}m2$ which are isomorphic to $\bar{3}2/m$; then by means of direct products one gets those of $6/m\;2/m\;2/m = \bar{3}2/m \otimes 2_c = 622 \otimes \bar{1} = 6mm \otimes \bar{1} = \bar{6}m2 \otimes \bar{1}$. The CRBs of 23 allow one to obtain those of $2/m\;\bar{3} = 23 \otimes \bar{1}$.

Concerning the group 432, it has been possible for us to obtain the CRBs of all subgroups except those of subgroups 1 and 2_{a+b} (or its conjugates). For both unique cases, the proposed method only enables one to get a partial reduction; it is possible to end the reduction by means of projection operators starting from an extensively reduced representation. By means of an isomorphy one gets the analogous CRBs of $\bar{4}3m$ and then by means of direct products one obtains those of $4/m\;\bar{3}2/m = 432 \otimes \bar{1} = \bar{4}3m \otimes \bar{1}$.

The CRBs of the non-equivalent PIRs of the groups $\bar{1}$, 4, 422, 3, 32, 23 and 432 are recorded in the deposit;* the CRBs of other groups may be deduced by isomorphy and direct products without difficulty. We remark that for *all* IRs of *all* crystallographic point groups a basis is available up to an equivalence.

The methods used in the present work extend to other groups, *i.e.* non-crystallographic point groups and especially to icosahedral groups I and I_h, to double groups (crystallographic or not) (see deposit) *etc.*

Lastly, note that for groups not so well known as the groups enumerated above, the proposed method allows one to gain access to their IRs and their characters when they are not known.

* Data for groups $\bar{1}$, 4, 422, 3, 32, 23 and 432 have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52841 (5 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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