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How to Obtain Easily the Induced Representations of Point Groups: the Icosahedral Point Groups

BY YVES BILLIET

Département de Chimie, Faculté des Sciences, Boîte Postale N° 825, Niamey, Niger

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Abstract

With tables of subduced representations as a starting point and use of the Frobenius reciprocity theorem, a simple method to obtain induced representations is given. Tables are given of the 22 induced representations of 532 (I) and of the 84 induced representations of $\bar{5}\bar{3}2/m$ (I_h).

Introduction

The crystallographic and molecular point groups are prime candidates to exemplify various group-theoretical properties. They are well known to both physicists and chemists. Their orders are not large so they lend themselves to non-computerized calculations but neither are they small so they can be used to illustrate the distinct possible cases of group-theoretical properties.

The properties we wish to emphasize here are those of subduced and induced representations of groups: their dimension, additivity, transitivity and how they are related by the Frobenius reciprocity theorem. These properties will be used to construct the induced representations of the icosahedral point groups 532 (I) and $\bar{5}\bar{3}2/m$ (I_h) from the subduced representations of these groups onto their subgroups.

We have chosen the icosahedral groups because of the interest in them in many fields: electronic (Boyle, 1972) and vibrational (Boyle & Parker, 1980) properties of molecules, coupling coefficients (Fowler & Ceulemans, 1985), the Jahn–Teller effect (Ceulemans & Fowler, 1989, 1990), inorganic (Pitochelli & Hawthorne, 1960) and biological molecules (Litvin, 1975), and quasicrystals (Schechtman, Blech, Gratias & Cahn, 1984; Jaric, 1988). Recently, Litvin (1991) tabulated many of the basic group-theoretical properties of the icosahedral point groups. Their irreducible representations and character tables are well known (Griffith, 1964; Backhouse & Gard, 1974). We do not give here the fundamental principles of group theory or group representations and instead refer the reader to classic works (Lomont, 1959; Murnagham, 1963; Gorenstein, 1968; Kirillov, 1976; Serre, 1978; Malliavin, 1981).

I. Notation and basic properties

Consider a finite group G, a subgroup H, a representation $\pi(G)$ of G and a representation $\rho(H)$ of H.

(i) The representation of H subduced from $\pi(G)$ is denoted $\pi(G)\downarrow H$, while the representation of G induced by $\rho(H)$ is denoted $\rho(H)\uparrow G$.

(ii) The dimensions of these representations are related:

$$\dim[\pi(G)\downarrow H] = \dim[\pi(G)];$$
$$\dim[\rho(H)\uparrow G] = \dim[\rho(H)]\times|G|/|H|;$$

where $|G|$ and $|H|$ are the orders of G and H, respectively.

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Table 1. *Representations of the subgroups subduced from the irreducible representations of the group* 532 (I)

Only one subgroup appears for each conjugation class. An asterisk (*) marks the two-dimensional reducible representations consisting of two complex-conjugate one-dimensional irreducible representations.

532	1	2	222	3	32	23	5	52
I	C_1	C_2	D_2	C_3	D_3	T	C_5	D_5
A	A	A	A	A	A_1	A	A	A_1
T_1	$3A$	$A+2B$	$B_1+B_2+B_3$	$A+E^*$	A_2+E	T	$A+E_1^*$	A_2+E_1
T_2	$3A$	$A+2B$	$B_1+B_2+B_3$	$A+E^*$	A_2+E	T	$A+E_2^*$	A_2+E_2
G	$4A$	$2A+2B$	$A+B_1+B_2+B_3$	$2A+E^*$	A_1+A_2+E	$A+T$	$E_1^*+E_2^*$	E_1+E_2
H	$5A$	$3A+2B$	$2A+B_1+B_2+B_3$	$A+2E^*$	A_1+2E	E^*+T	$A+E_1^*+E_2^*$	$A_1+E_1+E_2$

(iii) The character of $\pi(G)\downarrow H$ is equal to the character of $\pi(G)$ restricted to the elements of G belonging to H.

(iv) The trace of an element g of G in the character of $\rho(H)\uparrow G$ is given by

$$\chi[\rho(H)\uparrow G, g] = |H|^{-1} \sum \chi[\rho(H), sgs^{-1}],$$

where the sum is extended to those elements s of g for which sgs^{-1} belongs to H.

(v) The subduction and the induction possess the additivity property:

$$(\pi_1+\pi_2)(G)\downarrow H = \pi_1(G)\downarrow H + \pi_2(G)\downarrow H;$$

$$(\rho_1+\rho_2)(H)\uparrow G = \rho_1(H)\uparrow G + \rho_2(H)\uparrow G.$$

(vi) Consider an intermediate subgroup F, $H \subset F \subset G$. One has the transitivity property:

$$[\pi(G)\downarrow F]\downarrow H = \pi(G)\downarrow H;$$

$$[\rho(H)\uparrow F]\uparrow G = \rho(H)\uparrow G.$$

(vii) Finally, consider an irreducible representation $\pi^\circ(G)$ and an irreducible representation $\rho^\circ(H)$. The Frobenius reciprocity theorem states that the number of times $\pi^\circ(G)$ is contained in $\rho^\circ(H)\uparrow G$ is equal to the number of times $\rho^\circ(H)$ is contained in $\pi^\circ(G)\downarrow H$.

II. Construction of induced representations

It is relatively easy to obtain the subduced representations of a point group subduced onto its subgroups. The character table of a point group is used to obtain the character of the subduced representation. This representation is then reduced into its irreducible components, which is not too difficult. This has been done for all point groups and there exist numerous tables (correlation tables) of subduced representations (see, for example, Atkins, Child & Phillips, 1970; Pelikán & Breza, 1985; Salthouse & Ware, 1972). We reproduce in Table 1 the reduced form of the subduced representations of the icosahedral point group 532 (I).

To our knowledge, there is no systematic tabulation of induced representations of the point groups. It is possible to calculate the characters of the induced representations using property (iv) above, but this is not an efficient method as it requires knowledge of the point-group multiplication table and numerous calculations. However, it is relatively easy to construct the induced representations directly using property (vii) above, where one uses the tables of subduced representations and the Frobenius reciprocity theorem.

For example, let us determine the representation of 532 (I) induced by the representation $A+2B_3$ of 222 (D_2). Notice that it is necessary to start with the expression of $\rho(H)$ reduced into its irreducible components. From Table 1, we have that $A(222)$ appears once in $A(532)\downarrow 222$, once in $G(532)\downarrow 222$ and twice in $H(532)\downarrow 222$; and as a consequence of the Frobenius reciprocity theorem, $A(532)$ is contained once, $G(532)$ is contained once and $H(532)$ is contained twice in $A(222)\uparrow 532$. Thus, one has

$$\mathrm{A}(222)\uparrow 532 = A+G+2H,$$

$$\dim[A(222)]\times|532|/|222| = 1\times 60/4 = 15,$$

according to [*cf.* (ii)]

$$\dim[(A+G+2H)(532)] = 1+4+2\times 5 = 15.$$

In the same way, one has

$$B_3(222)\uparrow 532 = T_1+T_2+G+H,$$

$$\dim[B_3(222)]\times|532|/|222| = 1\times 60/4 = 15$$

and

$$\dim[(T_1+T_2+G+H)(532)] = 3+3+4+5 = 15.$$

Therefore, we conclude [*cf.* (v)] that

$$\begin{aligned}(A+2B_3)&(222)\uparrow 532\\ &= A(222)\uparrow 532 + 2B_3(222)\uparrow 532\\ &= A+2T_1+2T_2+3G+4H,\end{aligned}$$

$$\dim[(A+2B_3)(222)]\times|532|/|222| = 3\times 60/4 = 45,$$

which is consistent with

$$\begin{aligned}\dim&[(A+2T_1+2T_2+3G+4H)(532)]\\ &= 1+2\times 3+2\times 3+3\times 4+4\times 5 = 45.\end{aligned}$$

We have applied this process to tabulate in Tables 2 and 3 the irreducible components of all induced representations of, respectively, the icosahedral point groups 532 (I) and $\bar{5}\bar{3}2/m$ (I_h).

This process is very simple and yields the induced representations in a much-reduced expression. Nevertheless, there is a pitfall. Suppose that one wishes to get the representation of 532 (I) induced by the representation E of the subgroup 23 (T). From Table 1, one sees that $E(23)$ is contained only once in $H(532)$ and one may hastily conclude that

$$E(23)\uparrow 532 = H.$$

Table 2. *Representations of the group* 532 (I) *induced by the irreducible representations of its subgroups*

Conjugate subgroups induce equivalent representations. The correspondence between the International and Schoenflies notations of point groups is given in Table 1. Notation such as $\frac{1}{2}E(23)$: H occurs for the equivalent representations induced by each component of a two-dimensional reducible representation consisting of two complex-conjugate one-dimensional irreducible representations.

Note that one may verify from Tables 2 and 3 another property of the induced representations: if $\pi_{\rm reg}(G)$ and $\rho_{\rm reg}(H)$ are the regular representations of G and H, then $\rho_{\rm reg}(H)\uparrow G=\pi_{\rm reg}(G)$. Examples: $(A_1+A_2+2E)(32)\uparrow 532=A+3T_1+3T_2+4G+5H$; $(A+E+3T)(23)\uparrow \bar{5}\bar{3}2/m=A_g+3T_{1g}+3T_{2g}+4G_g+5H_g+A_u+3T_{1u}+3T_{2u}+4G_u+5H_u$.

$A(1)$:	$A+3T_1+3T_2+4G+5H$
$A(2)$:	$A+T_1+T_2+2G+3H$
$B(2)$:	$2T_1+2T_2+2G+2H$
$A(222)$:	$A+G+2H$
$B_1(222)$:	T_1+T_2+G+H
$B_2(222)$:	T_1+T_2+G+H
$B_3(222)$:	T_1+T_2+G+H
$A(3)$:	$A+T_1+T_2+2G+H$
$\frac{1}{2}E(3)$:	T_1+T_2+G+2H
$A_1(32)$:	$A+G+H$
$A_2(32)$:	T_1+T_2+G
$E(32)$:	T_1+T_2+G+2H
$A(23)$:	$A+G$
$\frac{1}{2}E(23)$:	H
$T(23)$:	T_1+T_2+G+H
$A(5)$:	$A+T_1+T_2+H$
$\frac{1}{2}E_1(5)$:	T_1+G+H
$\frac{1}{2}E_2(5)$:	T_2+G+H
$A_1(52)$:	$A+H$
$A_2(52)$:	T_1+T_2
$E_1(52)$:	T_1+G+H
$E_2(52)$:	T_2+G+H

Table 3. *Representations of the group* $\bar{5}\bar{3}2/m$ (I_h) *induced by the irreducible representations of its subgroups*

Conjugate subgroups induce equivalent representations. The correspondence between the international and Schoeflies notations of point groups is 1-C_1, $\bar{1}$-C_i, 2-C_2, m-C_s, 222-D_2, $mm2$-C_{2v}, $2/m\,2/m\,2/m$-D_{2h}, 3-C_3, $\bar{3}$-C_{3i} or S_6, 32-D_3, $3m$-C_{3v}, $\bar{3}2/m$-D_{3d}, 23-T, $2/m\bar{3}$-T_h, 5-C_5, $\bar{5}$-C_{5i} or S_{10}, 52-D_5, $5m$-C_{5v}, $\bar{5}2/m$-D_{5d}, 532-I. Notation such as $\frac{1}{2}E(23)$: H_g+H_u occurs for the equivalent representations induced by each component of a two-dimensional reducible representation consisting of two complex-conjugate one-dimensional irreducible representations.

$A(1)$:	$A_g+3T_{1g}+3T_{2g}+4G_g+5H_g$ $+A_u+3T_{1u}+3T_{2u}+4G_u+5H_u$
$A_g(\bar{1})$:	$A_g+3T_{1g}+3T_{2g}+4G_g+5H_g$
$A_u(\bar{1})$:	$A_u+3T_{1u}+3T_{2u}+4G_u+5H_u$
$A(2)$:	$A_g+T_{1g}+T_{2g}+2G_g+3H_g$ $+A_u+T_{1u}+T_{2u}+2G_u+3H_u$
$B(2)$:	$2T_{1g}+2T_{2g}+2G_g+2H_g$ $+2T_{1u}+2T_{2u}+2G_u+2H_u$
$A'(m)$:	$A_g+T_{1g}+T_{2g}+2G_g+3H_g$ $+2T_{1u}+2T_{2u}+2G_u+2H_u$
$A''(m)$:	$2T_{1g}+2T_{2g}+2G_g+2H_g$ $+A_u+T_{1u}+T_{2u}+2G_u+3H_u$
$A_g(2/m)$:	$A_g+T_{1g}+T_{2g}+2G_g+3H_g$
$B_g(2/m)$:	$2T_{1g}+2T_{2g}+2G_g+2H_g$
$A_u(2/m)$:	$A_u+T_{1u}+T_{2u}+2G_u+3H_u$
$B_u(2/m)$:	$2T_{1u}+2T_{2u}+2G_u+2H_u$

Table 3 (*cont.*)

$A(222)$:	$A_g+G_g+2H_g+A_u+G_u+2H_u$
$B_1(222)$:	$T_{1g}+T_{2g}+G_g+H_g+T_{1u}+T_{2u}+G_u+H_u$
$B_2(222)$:	$T_{1g}+T_{2g}+G_g+H_g+T_{1u}+T_{2u}+G_u+H_u$
$B_3(222)$:	$T_{1g}+T_{2g}+G_g+H_g+T_{1u}+T_{2u}+G_u+H_u$
$A_1(mm2)$:	$A_g+G_g+2H_g+T_{1u}+T_{2u}+G_u+H_u$
$A_2(mm2)$:	$T_{1g}+T_{2g}+G_g+H_g+A_u+G_u+2H_u$
$B_1(mm2)$:	$T_{1g}+T_{2g}+G_g+H_g+T_{1u}+T_{2u}+G_u+H_u$
$B_2(mm2)$:	$T_{1g}+T_{2g}+G_g+H_g+T_{1u}+T_{2u}+G_u+H_u$
$A_g(2/m\,2/m\,2/m)$:	$A_g+G_g+2H_g$
$B_{1g}(2/m\,2/m\,2/m)$:	$T_{1g}+T_{2g}+G_g+H_g$
$B_{2g}(2/m\,2/m\,2/m)$:	$T_{1g}+T_{2g}+G_g+H_g$
$B_{3g}(2/m\,2/m\,2/m)$:	$T_{1g}+T_{2g}+G_g+H_g$
$A_u(2/m\,2/m\,2/m)$:	$A_u+G_u+2H_u$
$B_{1u}(2/m\,2/m\,2/m)$:	$T_{1u}+T_{2u}+G_u+H_u$
$B_{2u}(2/m\,2/m\,2/m)$:	$T_{1u}+T_{2u}+G_u+H_u$
$B_{3u}(2/m\,2/m\,2/m)$:	$T_{1u}+T_{2u}+G_u+H_u$
$A(3)$:	$A_g+T_{1g}+T_{2g}+2G_g+H_g$ $+A_u+T_{1u}+T_{2u}+2G_u+H_u$
$\frac{1}{2}E(3)$:	$T_{1g}+T_{2g}+G_g+2H_g$ $+T_{1u}+T_{2u}+G_u+2H_u$
$A_g(\bar{3})$:	$A_g+T_{1g}+T_{2g}+2G_g+H_g$
$\frac{1}{2}E_g(\bar{3})$:	$T_{1g}+T_{2g}+G_g+2H_g$
$A_u(\bar{3})$:	$A_u+T_{1u}+T_{2u}+2G_u+H_u$
$\frac{1}{2}E_u(\bar{3})$:	$T_{1u}+T_{2u}+G_u+2H_u$
$A_1(32)$:	$A_g+G_g+H_g+A_u+G_u+H_u$
$A_2(32)$:	$T_{1g}+T_{2g}+G_g+T_{1u}+T_{2u}+G_u$
$E(32)$:	$T_{1g}+T_{2g}+G_g+2H_g$ $+T_{1u}+T_{2u}+G_u+2H_u$
$A_1(3m)$:	$A_g+G_g+H_g+T_{1u}+T_{2u}+G_u$
$A_2(3m)$:	$T_{1g}+T_{2g}+G_g+A_u+G_u+H_u$
$E(3m)$:	$T_{1g}+T_{2g}+G_g+2H_g$ $+T_{1u}+T_{2u}+G_u+2H_u$
$A_{1g}(\bar{3}2/m)$:	$A_g+G_g+H_g$
$A_{2g}(\bar{3}2/m)$:	$T_{1g}+T_{2g}+G_g$
$E_g(\bar{3}2/m)$:	$T_{1g}+T_{2g}+G_g+2H_g$
$A_{1u}(\bar{3}2/m)$:	$A_u+G_u+H_u$
$A_{2u}(\bar{3}2/m)$:	$T_{1u}+T_{2u}+G_u$
$E_u(\bar{3}2/m)$:	$T_{1u}+T_{2u}+G_u+2H_u$
$A(23)$:	$A_g+G_g+A_u+G_u$
$\frac{1}{2}E(23)$:	H_g+H_u
$T(23)$:	$T_{1g}+T_{2g}+G_g+H_g+T_{1u}+T_{2u}+G_u+H_u$
$A_g(2/m\bar{3})$:	A_g+G_g
$\frac{1}{2}E_g(2/m\bar{3})$:	H_g
$T_g(2/m\bar{3})$:	$T_{1g}+T_{2g}+G_g+H_g$
$A_u(2/m\bar{3})$:	A_u+G_u
$\frac{1}{2}E_u(2/m\bar{3})$:	H_u
$T_u(2/m\bar{3})$:	$T_{1u}+T_{2u}+G_u+H_u$
$A(5)$:	$A_g+T_{1g}+T_{2g}+H_g+A_u+T_{1u}+T_{2u}+H_u$
$\frac{1}{2}E_1(5)$:	$T_{1g}+G_g+H_g+T_{1u}+G_u+H_u$
$\frac{1}{2}E_2(5)$:	$T_{2g}+G_g+H_g+T_{2u}+G_u+H_u$
$A_g(\bar{5})$:	$A_g+T_{1g}+T_{2g}+H_g$
$\frac{1}{2}E_{1g}(\bar{5})$:	$T_{1g}+G_g+H_g$
$\frac{1}{2}E_{2g}(\bar{5})$:	$T_{2g}+G_g+H_g$
$A_u(\bar{5})$:	$A_u+T_{1u}+T_{2u}+H_u$
$\frac{1}{2}E_{1u}(\bar{5})$:	$T_{1u}+G_u+H_u$
$\frac{1}{2}E_{2u}(\bar{5})$:	$T_{2u}+G_u+H_u$
$A_1(52)$:	$A_g+H_g+A_u+H_u$
$A_2(52)$:	$T_{1g}+T_{2g}+T_{1u}+T_{2u}$
$E_1(52)$:	$T_{1g}+G_g+H_g+T_{1u}+G_u+H_u$
$E_2(52)$:	$T_{2g}+G_g+H_g+T_{2u}+G_u+H_u$
$A_1(5m)$:	$A_g+H_g+T_{1u}+T_{2u}$
$A_2(5m)$:	$T_{1g}+T_{2g}+A_u+H_u$
$E_1(5m)$:	$T_{1g}+G_g+H_g+T_{1u}+G_u+H_u$
$E_2(5m)$:	$T_{2g}+G_g+H_g+T_{2u}+G_u+H_u$
$A_{1g}(\bar{5}2/m)$:	A_g+H_g
$A_{2g}(\bar{5}2/m)$:	$T_{1g}+T_{2g}$
$E_{1g}(\bar{5}2/m)$:	$T_{1g}+G_g+H_g$
$E_{2g}(\bar{5}2/m)$:	$T_{2g}+G_g+H_g$
$A_{1u}(\bar{5}2/m)$:	A_u+H_u
$A_{2u}(\bar{5}2/m)$:	$T_{1u}+T_{2u}$
$E_{1u}(\bar{5}2/m)$:	$T_{1u}+G_u+H_u$
$E_{2u}(\bar{5}2/m)$:	$T_{2u}+G_u+H_u$
$A(532)$:	A_g+A_u
$T_1(532)$:	$T_{1g}+T_{1u}$
$T_2(532)$:	$T_{2g}+T_{2u}$
$G(532)$:	G_g+G_u
$H(532)$:	H_g+H_u

However, with application of property (ii), one calculates

$$\dim[E(23)]\times|532|/|23| = 2\times 60/12 = 10,$$

while

$$\dim[H(532)] = 5!$$

In fact, the theorem of Frobenius was wrongly used. This theorem is valid only for irreducible representations. The representation $E(23)$ is not irreducible; it is in fact the sum of two complex-conjugate irreducible representations of 23. The induced representation of each of them is indeed $H(532)$, so the correct answer is

$$E(23)\uparrow 532 = 2H.$$

On the other hand, if one considers the representation E of the subgroup 32 (D_3) of 532 (I), it is irreducible and one has (*cf.* Table 1)

$$E(32)\uparrow 532 = T_1 + T_2 + G + 2H,$$

$$\dim[E(32)]\times|532|/|32| = 2\times 60/6 = 20,$$

consistent with

$$\dim[(T_1 + T_2 + G + 2H)(532)]$$
$$= 3+3+4+2\times 5 = 20.$$

Finally, it is also possible to obtain the induced representations from a chain of subgroups using the transitivity property (vi). For example, consider the subgroup chain 532 (I)-23 (T)-222 (D_2)-2 (C_2) and the induced representation $B(2)\uparrow 532$. From tables of subduced representations (see, for example, Atkins, Child & Phillips, 1970), we have*

$$B(2)\uparrow 222 = B_2 + B_3,$$

$$(B_2 + B_3)(222)\uparrow 23 = 2T,$$

$$2T(23)\uparrow 523 = 2T_1 + 2T_2 + 2G + 2H$$

and, consequently, using the transitivity property (vi), we have

$$B(2)\uparrow 532 = 2T_1 + 2T_2 + 2G + 2H.$$

* In the first step of the induction, we have supposed that axis 2 has the direction **c** in 222. If axis 2 is supposed to have the direction **a** or the direction **b**, the first step leads to $B(2)\uparrow 222 = B_1 + B_2$ or $B_1 + B_3$. But each representation B_1, B_2 or B_3 of 222 induces a representation T of 23, so that the next steps of the induction remain identical in any case. Moreover, one notes that all axes 2 induce necessarily equivalent representations because they are conjugate in 532.

We have tabulated* the induced representations, using the Frobenius reciprocity theorem, of all 32 crystallographic point groups and the molecular point groups 5 (C_5), $\bar{5}$ [$C_{5i}(S_{10})$], 52 (D_2), $5m$ (C_{5v}), $\bar{5}2/m$ (D_{5d}), $\overline{10}$ (C_{5h}), $\overline{10}m2$ (D_{5h}), 532 (I) and $\bar{5}\bar{3}2/m$ (I_h).

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* Lists of induced representations of crystallographic and other molecular point groups have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55724 (48 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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