understood that more than one such term may be required, although typically examples used require only one. This section is intended to show the probabilities associated with the minimum necessary number of such terms in the triclinic case.

Since the same colour translation groups apply to the reciprocal lattice as to the direct lattice, their number and relative frequency will be given by the same formulae as above with the assumption that a typical data set is large enough for the asymptotic formulae to be closely approximated. We can also make the correlation that if a lattice belongs to a colour group comprising one cycle only it will require one co-opted term and if two cycles, two terms *etc.* However, the reciprocal sublattice imposed by the defining trio in the phase-determining process must be of odd index to resolve the origin ambiguity. In such a case we must eliminate the prime 2 from our formulae, by making use of the prime-product form

$$\zeta(s)=\prod_p(1-p^{-s})^{-1},$$

with any function $\zeta(s)$ replaced by

$$\prod_{p\neq 2}(1-p^{-s})^{-1} \quad \text{or} \quad (1-2^{-s})\zeta(s).$$

This is analogous to the handling of centred lattices by Rutherford (1992*b*). For example, while the proportion of all integers that are square-free is

$$\zeta^{-1}(2)=6/\pi^2=0.60792\ldots,$$

the proportion of odd integers that are square-free is

$$[(1-2^{-2})\zeta(2)]^{-1}=8/\pi^2=0.81057\ldots.$$

On this basis, the asymptotic average number of triclinic derivative lattices of odd index is

$$\tfrac{3}{4}\times\tfrac{7}{8}\zeta(2)\zeta(3)n^2$$

and, since the fraction of integers that are odd is $\frac{1}{2}$, the fraction of all lattices having odd index is

$$\tfrac{1}{2}\times\tfrac{3}{4}\times\tfrac{7}{8}\zeta(2)\zeta(3)n^2/\zeta(2)\zeta(3)n^2=\tfrac{1}{2}\times\tfrac{3}{4}\times\tfrac{7}{8}=0.328125.$$

Examination of the lower part of Table 2 shows that this ratio is approximated there.

To return to the co-opted terms, the expression $[\zeta(4)\zeta(9)]^{-1}$ becomes $(16/15)\times(512/511)[\zeta(4)\zeta(9)]^{-1}$ and $\zeta^{-1}(9)$ becomes $(512/511)\zeta^{-1}(9)$. When evaluated, these modified expressions give the ratio for the cases of a minimum of one co-opted term, or of two or of three, to be

$$0.98548:0.01447:0.00005.$$

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Representations of Point Groups Spanned by Sets of Equivalent Bipoints or Multipoints

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Abstract

The properties of the representations of the three-dimensional point groups spanned by sets of equivalent bipoints are studied (characters and reductions); these representations are either principal induced representations or monomial representations induced by the subgroups (stabilizer subgroups and

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extended stabilizer subgroups of the bipoints). The properties are also relevant to sets of equivalent tripoints or multipoints. Several examples and tables are given in the case of the point group $\bar{6}m2$. Applications are illustrated by some bipoint and multipoint representations of the cyclopropane molecule.

Introduction

The concept of the principal induced representations (PIRs) of a crystallographic group has recently been a subject of increasing interest and several papers have been devoted to the properties and applications of PIRs (Litvin, 1982; Berenson, Kotzev & Litvin, 1982; Litvin, Kotzev & Birman, 1982; Masmoudi, 1990; Masmoudi & Billiet, 1989, 1990*a*, *b*). The PIRs of a group belong to a more extended category of representations designated as monomial representations (MRs).

In the present work, the properties of PIRs and MRs are applied to the study of the representations of point groups that are spanned by sets of equivalent bipoints or of equivalent multipoints.

For details of the well known mathematical definitions and properties mentioned in this paper, the reader is referred to the classic works (Gorenstein, 1968; Kirillov, 1976; Lomont, 1959; Malliavin, 1981; Murnagham, 1963; Serre, 1978). For other more specialized items and demonstrations, reference is made to Masmoudi (1990) and Masmoudi & Billiet (1989, 1990*a*).

I. Notation

Consider a point group G and a subgroup K. The representation of G spanned by the cosets of the left partition of G with respect to K is a PIR of G denoted by $R(K\uparrow G)$ or $R(K)$ if no confusion is possible; this representation may also be defined as the representation of G induced by the identity representation of K (whose traces are all equal to $+1$). The trace of an element g of G in this PIR is given by

$$\chi[R(K\uparrow G), g] = p_K c_K(g)/c_K,$$

where p_K is the index of K in G, c_K is the number of subgroups of G conjugate to K and $c_K(g)$ is the number of those subgroups containing g.

The weight of the irreducible representation R_α of G in $R(K\uparrow G)$ is given by

$$m_K(R_\alpha) = (1/|K|)\sum_{k\in K}\chi(R_\alpha, k),$$

where $|K|$ is the order of K.

Consider now an alternating representation $D(F)$ of a subgroup F of G, that is to say a one-dimensional representation of F whose traces are either $+1$ or -1, with equal probability. The representation of G induced by $D(F)$ is a MR denoted $M[D(F)\uparrow G]$ or, more briefly, $M[D(F)]$ if there is no confusion. The next direct-sum property (Masmoudi, 1990) holds,

$$R(H\uparrow G) = R(F\uparrow G) + M[D(F)\uparrow G].$$

Here H is the subgroup of index 2 of F whose traces are all equal to $+1$ in $D(F)$. Then $M[D(F)\uparrow G]$ is equivalently defined by the direct-difference relation,

$$M[D(F)\uparrow G] = R(H\uparrow G) - R(F\uparrow G).$$

This relation stems from the fact that the characters of these representations are related by the equivalent properties:

$$\chi R(H\uparrow G) = \chi R(F\uparrow G) + \chi M[D(F)\uparrow G];$$

$$\chi M[D(F)\uparrow G] = \chi R(H\uparrow G) - \chi R(F\rightarrow G).$$

Consider now two distinct points A and B of the crystallographic space, the bipoint (A, B) that they define and an element g of G. If and only if g transforms the point A into the point C and the point B into the point D, we say 'g transforms the bipoint (A, B) into the bipoint (C, D)' and we write $g(A, B) = (C, D)$. We say 'g reverses (A, B)' if $g(A, B) = (B, A)$ and we write $g(A, B) = -(A, B)$.

We define the stabilizer subgroup of (A, B) as the subgroup G' of G leaving (A, B) invariant [$\forall g' \in G'$, $g'(A, B) = (A, B)$]. Finally, we define the extended stabilizer subgroup of (A, B) as the subgroup G'' of G whose elements either leave (A, B) invariant or reverse (A, B) [$\forall g'' \in G''$, $g''(A, B) = (A, B)$ or $g''(A, B) = -(A, B)$, *i.e.* $g''(A, B) = \pm(A, B)$]. Note that G' is a subgroup of index 2 of G''; alternatively it may be identical with G''.

II. Bipoint representations

We consider two bipoints (A, B) and (C, D) as equivalent if and only if there exists at least one element g of G such that $g(A, B) = \pm(C, D)$. Now consider the set $\{(A, B)\}$ of bipoints equivalent to (A, B) (note that, in listing the elements of this set, we make no distinction between a bipoint and its reverse). This set spans a representation $R(A, B)$ of G, a so-called 'bipoint representation',* the dimension of which is the number of distinct bipoints of $\{(A, B)\}$. Two cases may be distinguished.

* To avoid confusion, we have not used the term 'vector' in this paper. The elements $(A, B), (C, D), \ldots$ of the set $\{(A, B)\}$ are really vectors of the vector space Λ of the representation $R(A, B)$; they constitute in fact a basis of the representation $R(A, B)$, so they are independent in Λ. But to each bipoint $(A, B), (C, D), \ldots$ of the crystallographic *affine* space corresponds a vector **AB**, **CD**, ... of the associated *vector* space. These vectors are not necessarily independent. For instance, consider the six equivalent points $A(x, \bar{x}, z)$, $B(x, 2x, z)$, $C(2\bar{x}, \bar{x}, z)$, $D(x, \bar{x}, \bar{z})$, $E(x, 2x, \bar{z})$, $F(2\bar{x}, \bar{x}, \bar{z})$ of $\bar{6}m2$. The three bipoints (A, D), (B, E), (C, F) are independent and constitute a basis for the representation $A_2'' + E''$ of $\bar{6}m2$. But the three vectors **AD**, **BE**, **CF** are not independent: **AD** = **BE** = **CF**. Masmoudi (1990) gives another approach.

1. *No element of G reverses the bipoints*

In this case, the extended stabilizer subgroup of (A, B) is identical to the stabilizer subgroup H of (A, B). The trace of the element g of G in $R(A, B)$ is equal to the number of equivalent bipoints left invariant by g and consequently $R(A, B) = R(H\uparrow G)$. This is always the case when A and B are not equivalent, *i.e.* do not belong to the same set of equivalent points of G.

Example 1. Consider the point group $G = \bar{6}m2$ (Table 1) and take as points A and B the generators respectively of a set n and of a set g.

$$A{:}\ x_A, \bar{x}_A, z_A; \qquad B{:}\ 0, 0, z_B;$$

$$(A, B) = (x_A, \bar{x}_A, z_A; 0, 0, z_B) \text{ denoted } U_1;$$

$$H = m_{-a-b}.$$

The set of bipoints equivalent to (A, B) contains six elements:

$$\begin{aligned} &U_1; \\ &U_2 = (x_A, 2x_A, z_A; 0, 0, z_B); \\ &U_3 = (2\bar{x}_A, \bar{x}_A, z_A; 0, 0, z_B); \\ &U_4 = (x_A, \bar{x}_A, \bar{z}_A; 0, 0, \bar{z}_B); \\ &U_5 = (x_A, 2x_A, \bar{z}_A; 0, 0, \bar{z}_B); \\ &U_6 = (2\bar{x}_A, \bar{x}_A, \bar{z}_A; 0, 0, \bar{z}_B). \end{aligned}$$

The representation $R(A, B)$ is constructed, as follows. Suppose the symmetry operation m_b^1 of G: $m_b^1(U_1) = U_2$, $m_b^1(U_2) = U_1$, $m_b^1(U_3) = U_3$, $m_b^1(U_4) = U_5$, $m_b^1(U_5) = U_4$, $m_b^1(U_6) = U_6$. The matrix of m_b^1 in $R(A, B)$ is

$$\left|\begin{matrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{matrix}\right|.$$

The trace of the matrix of m_b^1 in $R(A, B)$ is $\chi[R(A, B), m_b^1] = 2$, *i.e.* is equal to the number of equivalent bipoints left invariant by m_b^1. By applying this process to the 12 elements of G, one obtains the character of $R(A, B)$:

g	1^1	3^1 3^2	m_a^1 m_b^1 m_{-a-b}^1	m_c^1	$\bar{6}^1$ $\bar{6}^5$	2^1_{a+2b} 2^1_{-2a-b} 2^1_{a-b}
$\chi[R(A, B), g]$	6	0	2	0	0	0

The reduction of $R(A, B)$ is as follows (*cf.* Tables 2, 3):

$$R(A, B) = A_1' + E' + A_2'' + E'' = R(m_{-a-b}\uparrow\bar{6}m2).$$

Table 1. *Sets of equivalent points of the point group* $\bar{6}m2$

The notation is directly derived from that of the space group $P\bar{6}m2$, No. 187 (*International Tables for Crystallography*, 1987); the coordinates are given with respect to the trigonal standard setting.

12	(o)	1	$x, y, z;\ \bar{y}, x-y, z;\ \bar{x}+y, \bar{x}, z;$ $x, y, \bar{z};\ \bar{y}, x-y, \bar{z};\ \bar{x}+y, \bar{x}, \bar{z};$ $\bar{y}, \bar{x}, z;\ \bar{x}+y, y, z;\ x, x-y, z;$ $\bar{y}, \bar{x}, \bar{z};\ \bar{x}+y, y, \bar{z};\ x, x-y, \bar{z}$
6	(n)	m	$x, \bar{x}, z;\ x, 2x, z;\ 2\bar{x}, \bar{x}, z;$ $x, \bar{x}, \bar{z};\ x, 2x, \bar{z};\ 2\bar{x}, \bar{x}, \bar{z}$
6	(l)	m	$x, y, 0;\ \bar{y}, x-y, 0;\ \bar{x}+y, \bar{x}, 0;$ $\bar{y}, \bar{x}, 0;\ \bar{x}+y, y, 0;\ x, x-y, 0$
3	(j)	$mm2$	$x, \bar{x}, 0;\ x, 2x, 0;\ 2\bar{x}, \bar{x}, 0$
2	(g)	$3m$	$0, 0, z;\ 0, 0, \bar{z}$
1	(a)	$\bar{6}m2$	$0, 0, 0$

Table 2. *Characters of the irreducible representations of the point group* $\bar{6}m2$

	1^1	2×3^1	$3\times m_a^1$	m_c^1	$2\times\bar{6}^1$	$3\times 2^1_{a+2b}$
A_1'	1	1	1	1	1	1
A_2'	1	1	−1	1	1	−1
E'	2	−1	0	2	−1	0
A_2''	1	1	1	−1	−1	−1
A_1''	1	1	−1	−1	−1	1
E''	2	−1	0	−2	1	0

Table 3. *Principal induced representations of the point group* $\bar{6}m2$

In each case, the inductor subgroup and the irreducible components have been recorded. The PIRs induced by two conjugate subgroups are equivalent, *i.e.* have the same irreducible components. The symbols of irreducible components refer to Table 2.

$$\begin{aligned} R(1) &= A_1' + A_2' + 2E' + A_2'' + A_1'' + 2E'' \\ R(2_{a+2b}) &= A_1' + E' + A_2'' + E'' \\ R(m_a) &= A_1' + E' + A_2'' + E'' \\ R(m_c) &= A_1' + A_2' + 2E' \\ R(3) &= A_1' + A_2' + A_2'' + A_1'' \\ R(m_c m_a 2_{a+2b}) &= A_1' + E' \\ R(32) &= A_1' + A_1'' \\ R(3m) &= A_1' + A_2'' \\ R(\bar{6}) &= A_1' + A_2' \\ R(\bar{6}m2) &= A_1' \end{aligned}$$

In the next example, we will see that one again obtains $R(A, B) = R(H\uparrow G)$, even though A and B belong to the same set of equivalent points of G, provided that no element of G simultaneously transforms A into B and B into A.

Example 2. Consider again the point group $G = \bar{6}m2$ (Table 1) and take A and B in the same set l as follows:

$$A{:}\ x_A, y_A, 0; \qquad B{:}\ \bar{y}_A, x_A - y_A, 0;$$

$$(A, B) = U_1 = (x_A, y_A, 0; \bar{y}_A, x_A - y_A, 0);$$

$$H = m_c.$$

The set $\{(A, B)\}$ contains six elements:

$$U_1;$$
$$U_2 = (\bar{y}_A, x_A - y_A, 0; \bar{x}_A + y_A, \bar{x}_A, 0);$$
$$U_3 = (\bar{x}_A + y_A, \bar{x}_A, 0; x_A, y_A, 0);$$
$$U_4 = (\bar{y}_A, \bar{x}_A, 0; \bar{x}_A + y_A, y_A, 0);$$
$$U_5 = (\bar{x}_A + y_A, y_A, 0; x_A, x_A - y_A, 0);$$
$$U_6 = (x_A, x_A - y_A, 0; \bar{y}_A, \bar{x}_A, 0).$$

Performing the construction of $R(A, B)$ as above, we obtain its character:

g	1^1	2×3^1	$3\times m_a^1$	m_c^1	$2\times \bar{6}^1$	$3\times 2^1_{a+2b}$
$\chi[R(A, B), g]$	6	0	0	6	0	0

The reduction of $R(A, B)$ leads to (*cf.* Tables 2, 3)

$$R(A, B) = A_1' + A_2' + 2E' = R(m_c \uparrow \bar{6}m2).$$

2. *Some elements of G reverse the bipoints*

In this event, the stabilizer subgroup H of (A, B) is a subgroup of index 2 of the extended stabilizer subgroup F of (A, B). The trace of the element g of G in $R(A, B)$ is equal to the number of bipoints left invariant by g reduced by the number of bipoints reversed by g. One has (Masmoudi, 1990):

$$R(A, B) = M[D(F)\uparrow G] = R(H\uparrow G) - R(F\uparrow G).$$

A and B necessarily belong to the same set of equivalent points of G and there exists at least one element of G that at the same time transforms A into B and B into A.

Example 3. $G = \bar{6}m2$. A and B belong to the same set l (*cf.* Table 1).

$$A\colon x_A, y_A, 0; \qquad B\colon \bar{y}_A, \bar{x}_A, 0; \qquad H = m_c;$$
$$F = m_c m_{-a-b} 2_{a-b}.$$

The set of bipoints equivalent to (A, B) contains three elements:

$$U_1 = (A, B) = (x_A, y_A, 0; \bar{y}_A, \bar{x}_A, 0);$$
$$U_2 = (\bar{y}_A, x_A - y_A, 0; x_A, x_A - y_A, 0);$$
$$U_3 = (\bar{x}_A + y_A, \bar{x}_A, 0; \bar{x}_A + y_A, y_A, 0).$$

The symmetry operation m_b^1 of G transforms the equivalent points as follows:

$$m_b^1(U_1) = -U_2;\ m_b^1(U_2) = -U_1;\ m_b^1(U_3) = -U_3;$$

thus, $\chi[R(A, B), m_b^1] = -1$. For the 12 elements of G, we have

g	1^1	2×3^1	$3\times m_a^1$	m_c^1	$2\times \bar{6}^1$	$3\times 2^1_{a+2b}$
$\chi[R(A, B), g]$	3	0	−1	3	0	−1

The reduction of $R(A, B)$ (*cf.* Tables 2, 3) is

$$R(A, B) = A_2' + E' = (A_1' + A_2' + 2E') - (A_1' + E')$$
$$= R(m_c \uparrow \bar{6}m2) - R(m_c m_{-a-b} 2_{a-b} \uparrow \bar{6}m2)$$
$$= M[B_2(m_c m_{-a-b} 2_{a-b}) \uparrow \bar{6}m2].$$

The MR of $\bar{6}m2$ is induced by the alternating representation B_2 of $m_c m_{-a-b} 2_{a-b}$ whose traces are respectively $\chi(1^1) = \chi(m_c^1) = 1$ and $\chi(m^1_{-a-b}) = \chi(2^1_{a-b}) = -1$.

The bipoint (A, B) that we have considered is in fact *oriented*, since some suitable symmetry operations g^0 are able to reverse it: $g^0(A, B) = (B, A) = -(A, B)$. We consider now the *nonoriented* bipoint $|A, B|$ associated with the oriented bipoint (A, B) and we write $g|A, B| = |A, B|$ if $g(A, B) = \pm(A, B)$. Thus the stabilizer subgroup of $|A, B|$ is identical to the extended stabilizer subgroup F of (A, B). Then we define the set $\{|A, B|\}$ of nonoriented bipoints equivalent to $|A, B|$ and the representation $R|A, B|$ spanned by this set in a similar way as for oriented bipoints. $R|A, B|$ is a PIR: $R|A, B| = R(F\uparrow G)$. Compare this with $R(A, B)$, which is a MR. $R(A, B) = R(H\uparrow G) - R(F\uparrow G)$.

Note that if no symmetry operation of G reverses (A, B) then $R(A, B) = R|A, B|$. In all cases, $\chi[R|A, B|, g] = |\chi[R(A, B), g]|$:

Example 3 (*cont.*).

g	1^1	2×3^1	$3\times m_a^1$	m_c^1	$3\times \bar{6}^1$	$3\times 2^1_{a+2b}$
$\chi[R\vert A, B\vert, g]$	3	0	1	3	0	1

$$R|A, B| = A_1' + E' = R(m_c m_{-a-b} 2_{a-b} \uparrow \bar{6}m2).$$

Such a procedure may be performed on all bipoints (oriented or not) whose constituents are taken in two sets (distinct or not) of equivalent points for all three-dimensional point groups. As an example, we give the complete list of spanned representations in the case of the point group $\bar{6}m2$ (Table 4).

III. Multipoint representations

Let A, B, C be three distinct points of crystallographic space. We say that the symmetry operation g transforms the tripoint (A, B, C) onto itself if g leaves invariant each point A, B, C or if g realizes an even permutation of the three points. Likewise we say that the symmetry operation g reverses the oriented tripoint (A, B, C) if g realizes an odd permutation of its points. The definitions of stabilizer subgroup H and extended stabilizer subgroup F are the same as for bipoints. Now consider two tripoints (A, B, C) and (D, E, F); we say that the symmetry operation g transforms (A, B, C) into (D, E, F) if $g(A) = D$, $g(B) = E$, $g(C) = F$ up to an even permutation and we write $g(A, B, C) = (D, E, F)$. If g transforms A, B, C in D, E, F up to an odd permutation we write

Table 4. *Representations of the point group $\bar{6}m2$ spanned by sets of equivalent bipoints*

The PIRs refer to Table 3. The Wyckoff types refer to Table 1 and the coordinates x, y, z have the usual meaning (see *International Tables for Crystallography*, 1987). The notation o-n means the set of bipoints equivalent to the bipoint of which the first point is any point of a set of equivalent points of Wyckoff type (o) and the second point is any point of a set of type (n). In the same way, j-j relates to a bipoint for which the points are any two distinct points of the same set of type (j). l_1-l_2 refers to a bipoint for which the first point is any point of a set of type (l) and the second point is any point of a second (distinct) set of type (l). When the points of the bipoint are not arbitrary, their coordinates are indicated, as in $o(x, y, z)$-$o(\bar{y}, \bar{x}, \bar{z})$ or $n_1(x_1, \bar{x}_1, z_1)-n_2(x_2, 2x_2, z_2)$; in this last case there is no relation connecting x_1 to x_2 and z_1 to z_2 but it is forbidden to have $x_1 = x_2$ and $z_1 = z_2$ simultaneously. However, the notation $n(x_1, \bar{x}_1, z_1)$-$j(x_2, 2x_2, 0)$ signifies that there is no relation connecting x_1 to x_2 but $x_1 = x_2$ is not forbidden. For bipoints that may be reversed by some elements of $\bar{6}m2$, two representations are given: the first is the MR spanned by the oriented bipoint, the second is the PIR spanned by the nonoriented bipoint.

o_1-o_2: $R(1)$
$o(x, y, z)$-$o(\bar{y}, x-y, z)$: $R(1)$
$o(x, y, z)$-$o(\bar{y}, x-y, \bar{z})$: $R(1)$
$o(x, y, z)$-$o(x, y, \bar{z})$: $R(1)-R(m_c) = M[A''(m_c)]$; $R(m_c)$
$o(x, y, z)$-$o(\bar{y}, \bar{x}, z)$: $R(1)-R(m_{-a-b}) = M[A''(m_{-a-b})]$; $R(m_{-a-b})$
$o(x, y, z)$-$o(\bar{y}, \bar{x}, \bar{z})$: $R(1)-R(2_{a-b}) = M[B(2_{a-b})]$; $R(2_{a-b})$
o-n: $R(1)$
o-l: $R(1)$
o-j: $R(1)$
o-g: $R(1)$
o-a: $R(1)$
$n_1(x_1, \bar{x}_1, z_1)$-$n_2(x_2, \bar{x}_2, z_2)$: $R(m_{-a-b})$
$n_1(x_1, \bar{x}_1, z_1)$-$n_2(x_2, 2x_2, z_2)$: $R(1)$
$n(x, \bar{x}, z)$-$n(x, 2x, z)$: $R(1)-R(m_b) = M[A''(m_b)]$; $R(m_b)$
$n(x, \bar{x}, z)$-$n(x, \bar{x}, \bar{z})$: $R(m_{-a-b})-R(m_c m_{-a-b} 2_{a-b})$
$= M[B_1(m_c m_{-a-b} 2_{a-b})]$; $R(m_c m_{-a-b} 2_{a-b})$
$n(x, \bar{x}, z)$-$n(x, 2x, \bar{z})$: $R(1)-R(2_{-2a-b}) = M[B(2_{-2a-b})]$; $R(2_{-2a-b})$
n-l: $R(1)$
$n(x_1, \bar{x}_1, z_1)$-$j(x_2, \bar{x}_2, 0)$: $R(m_{-a-b})$
$n(x_1, \bar{x}_1, z_1)$-$j(x_2, 2x_2, 0)$: $R(1)$
n-g: $R(m_{-a-b})$
n-a: $R(m_{-a-b})$
l_1-l_2: $R(m_c)$
$l(x, y, 0)$-$l(\bar{y}, x-y, 0)$: $R(m_c)$
$l(x, y, 0)$-$l(\bar{y}, \bar{x}, 0)$: $R(m_c) - R(m_c m_{-a-b} 2_{a-b})$
$= M[B_2(m_c m_{-a-b} 2_{a-b})]$; $R(m_c m_{-a-b} 2_{a-b})$
l-j: $R(m_c)$
l-g: $R(1)$
l-a: $R(m_c)$
$j_1(x_1, \bar{x}_1, 0)$-$j_2(x_2, \bar{x}_2, 0)$: $R(m_c m_{-a-b} 2_{a-b})$
$j_1(x_1, \bar{x}_1, 0)$-$j_2(x_2, 2x_2, 0)$: $R(m_c)$
j-j: $R(m_c)-R(m_c m_{-a-b} 2_{a-b}) = M[B_2(m_c m_{-a-b} 2_{a-b})]$; $R(m_c m_{-a-b} 2_{a-b})$
j-g: $R(m_{-a-b})$
j-a: $R(m_c m_{-a-b} 2_{a-b})$
g_1-g_2: $R(3m)$
g-g: $R(3m) - R(\bar{6}m2) = M[A_2''(\bar{6}m2)]$; $R(\bar{6}m2)$
g-a: $R(3m)$

$g(A, B, C) = -(D, E, F)$. The definitions and the properties of equivalent tripoints, set of equivalent tripoints and representations spanned by such a set are essentially the same as for bipoints. The same is true for nonoriented tripoints.

Example 4. As an application, consider the cyclopropane molecule C_3H_6, the point group of which is $\bar{6}m2$; the three C atoms [Wyckoff type (j), Table 1] and the six H atoms [Wyckoff type (n)] are respectively labelled A, B, C and D, E, F, G, H, I (Fig. 1). In Tables 5 and 6, some bipoint and tripoint rep-

Table 5. *Characters of some oriented or nonoriented bipoint or tripoint representations of the molecule of cyclopropane*

	1^1	2×3^1	$3\times m_a^1$	m_c^1	$2\times\bar{6}^1$	$3\times 2_{a+2b}^1$
$R(A, D)$	6	0	2	0	0	0
$R(D, E)$	6	0	−2	0	0	0
$R\|D, E\|$	6	0	2	0	0	0
$R(A, B)$	3	0	−1	3	0	−1
$R\|A, B\|$	3	0	1	3	0	1
$R(A, D, G)$	3	0	1	−3	0	−1
$R\|A, D, G\|$	3	0	1	3	0	1
$R(A, B, E)$	12	0	0	0	0	0
$R(D, E, F)$	2	2	−2	0	0	0
$R\|D, E, F\|$	2	2	2	0	0	0
$R(A, B, C)$	1	1	−1	1	1	−1
$R\|A, B, C\|$	1	1	1	1	1	1

resentations built on the atoms of this molecule are given.

All considerations apply to both oriented and nonoriented multipoints. However, when the number of points of the multipoints is greater than three, an extra juncture appears because there may be several ways to construct an oriented multipoint (or its reverse) starting from a given nonoriented multipoint.

Example 5. Consider the cyclopropane molecule (Fig. 1) and the nonoriented multipoint $|D, E, G, H|$, for which the stabilizer subgroup is $m_c m_b 2_{-2a-b}$. The PIR spanned by this multipoint and its equivalents is $R(m_c m_b 2_{-2a-b} \uparrow \bar{6}m2) = A_1' + E'$. There are three ways to obtain an oriented multipoint associated with

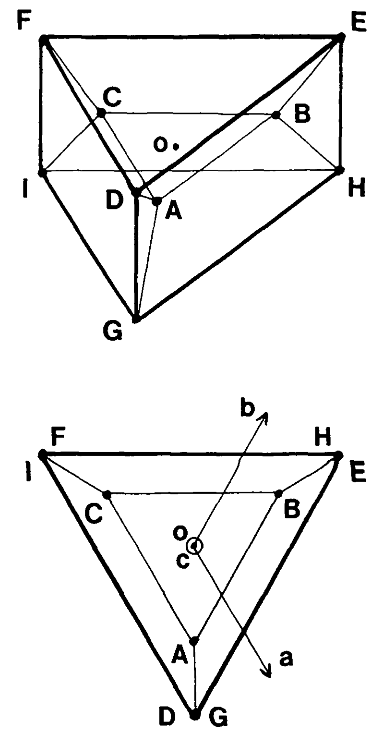

Fig. 1. The cyclopropane molecule: perspective and plan viewpoints.

Table 6. *Some oriented and nonoriented bipoint and tripoint representations of* C_3H_6 *as PIRs and MRs of the point group* $\bar{6}m2$

$$R(A, D) = R(m_{-a-b})$$
$$R(D, E) = R(1) - R(m_b) = M[A''(m_b)]$$
$$R|D, E| = R(m_b)$$
$$R(A, B) = R(m_c) - R(m_c m_b 2_{-2a-b}) = M[B_2(m_c m_b 2_{-2a-b})]$$
$$R|A, B| = R(m_c m_b 2_{-2a-b})$$
$$R(A, D, G) = R(m_{-a-b}) - R(m_c m_{-a-b} 2_{a-b}) = M[B_1(m_c m_{-a-b} 2_{a-b})]$$
$$R|A, D, G| = R(m_c m_{-a-b} 2_{a-b})$$
$$R(A, B, E) = R(1)$$
$$R(D, E, F) = R(3) - R(3m) = M[A_2(3m)]$$
$$R|D, E, F| = R(3m)$$
$$R(A, B, C) = R(\bar{6}) - R(\bar{6}m2) = M[A_2'(\bar{6}m2)]$$
$$R|A, B, C| = R(\bar{6}m2)$$

$|D, E, G, H|$; they are illustrated in Fig. 2, where the orientations are shown by arrows. For the first case, the stabilizer subgroup is m_b and the MR spanned by the oriented multipoint and its equivalents is (*cf.* Tables 2, 3):

$$R(m_b \uparrow \bar{6}m2) - R(m_c m_b 2_{-2a-b} \uparrow \bar{6}m2)$$
$$= M[B_1(m_c m_b 2_{-2a-b}) \uparrow \bar{6}m2]$$
$$= A_2'' + E''.$$

As to the second case, the stabilizer subgroup is m_c and the spanned representation is (*cf.* Tables 2 and 3)

$$R(m_c \uparrow \bar{6}m2) - R(m_c m_b 2_{-2a-b} \uparrow \bar{6}m2)$$
$$= M[B_2(m_c m_b 2_{-2a-b}) \uparrow \bar{6}m2]$$
$$= A_2' + E'.$$

In the last case, the stabilizer subgroup is 2_{-2a-b} and the spanned representation is (*cf.* Tables 2 and 3)

$$R(2_{-2a-b} \uparrow \bar{6}m2) - R(m_c m_b 2_{-2a-b} \uparrow \bar{6}m2)$$
$$= M[A_2(m_c m_b 2_{-2a-b}) \uparrow \bar{6}m2]$$
$$= A_1'' + E''.$$

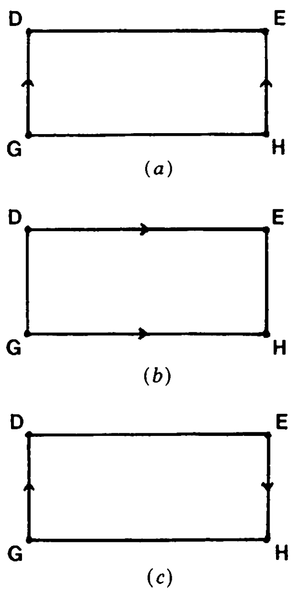

Fig. 2. Three ways to obtain an oriented multipoint starting from the nonoriented multipoint $|D, E, G, H|$. (*a*) The stabilizer subgroup is m_b. (*b*) The stabilizer subgroup is m_c. (*c*) The stabilizer subgroup is 2_{-2a-b}.

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