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Irreducible representations of the symmetry groups of polymer molecules II

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Abstract. The line groups are the symmetry groups of stereoregular polymer molecules. For quantum-mechanical applications one needs their unitary irreducible representations (reps). All reps of the line groups whose isogonal point groups are D_{nd} and D_{nh} ($n = 1, 2, 3, \dots$) are constructed. These reps are derived (directly or by induction) from those of the corresponding invariant subgroups of index two, which are the line groups with isogonal point groups C_{nv} . This paper, together with that by Božović, Vujičić and Herbut, gives the reps of all the line groups.

1. Introduction

From a study of the symmetries of stereoregular polymer molecules we constructed the line groups (Vujičić *et al* 1977, to be referred to as LG) which describe the symmetries of three-dimensional objects translationally periodical along a line. Stereoregular polymers are represented by such a model in most theoretical studies.

We also derived all the unitary irreducible representations (reps) for the line groups whose isogonal point groups are C_n , C_{nv} , C_{nh} , S_{2n} and D_n , $n = 1, 2, 3, \dots$ (Božović *et al* 1978, to be referred to as I). In this paper we complete the task by deriving the reps for the remaining line groups whose isogonal point groups are D_{nd} and D_{nh} , $n = 1, 2, 3, \dots$

The relevance of the line groups and their reps for physics of polymer molecules was discussed briefly in LG and I. One should perhaps add two novel facts concerning the band-structure theory of polymers. First, successful contacts have been made recently between theoretical predictions and x-ray photo-electron spectroscopy experiments (Delhalle 1980). The importance of conformation and symmetry was recognised in this context. Second, some line-group-theoretical arguments have been, for the first time, successfully incorporated into a band-structure computing system (Blumen and Merkel 1977, Ladik 1978), considerably improving the numerical behaviour of the system.

Apart from the $L2_1/mcm$ line group (Tobin 1955, McCubbin 1975) the reps of the line groups isogonal to D_{nd} or D_{nh} have not been studied before, although there are many polymer crystals known to belong to such crystal classes: e.g. poly(1-butene), poly(styrene) and poly(methylvinyl ether) belong to D_{3d} , while poly(vinyl cyclopentane) was found in D_{4h} and poly(oxymethylene) in the D_{6h} class (Miller 1975).

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2. Method of construction of reps

Every line group \mathbf{L} has an invariant subgroup \mathbf{T} consisting of a primitive translation and all its integral multiples. (In practice \mathbf{T} is usually made finite through cyclic boundary conditions (cf I); hence one can use the theory of finite groups.) The factor group \mathbf{L}/\mathbf{T} is isomorphic to the point group \mathbf{P} isogonal to \mathbf{L} .

The line groups considered in this paper are all of the form

$$\mathbf{L}^- = \mathbf{L}^+ + (R^-|0)\mathbf{L}^+ \quad (1)$$

where \mathbf{L}^+ is one of the line groups isogonal to one of the \mathbf{C}_{nv} point groups:

$$\mathbf{L}^+/\mathbf{T} \cong \mathbf{C}_{nv} \quad n = 1, 2, 3, \dots \quad (2)$$

Furthermore,

$$R^- = U_d \quad \text{when } \mathbf{L}^-/\mathbf{T} \cong \mathbf{D}_{nd} \quad (3)$$

while

$$R^- = \sigma_h \quad \text{when } \mathbf{L}^-/\mathbf{T} \cong \mathbf{D}_{nh}. \quad (4)$$

Here, U_d is a rotation through π around a horizontal axis forming the angle $\pi/2n$ with the vertical mirror plane σ_v and σ_h is the reflection in the horizontal plane. Both U_d and σ_h are involutions:

$$U_d^2 = \sigma_h^2 = E \quad (5)$$

where E is the identical operation. Consequently,

$$(R^-|0)^2 = (E|0), \quad (6)$$

so that each \mathbf{L}^- considered is a semi-direct product of its invariant subgroup \mathbf{L}^+ and the two-element subgroup generated by $(R^-|0)$:

$$\mathbf{L}^- = \mathbf{L}^+ \wedge \mathbf{J} \quad (7)$$

where $\mathbf{J} = \{(E|0), (R^-|0)\}$. Using this fact, one can construct all the reps of \mathbf{L}^- from the reps of \mathbf{L}^+ .

Let $\bar{D}(R^+|v+t) \equiv D[(R^-|0)(R^+|v+t)(R^-|0)^{-1}]$ be the rep of \mathbf{L}^+ conjugate by $(R^-|0)$ to $D(R^+|v+t)$, where R^+ is either C_n^s or $\sigma_v C_n^s$, $s = 0, 1, \dots, n-1$ and v equals 0 or $\frac{1}{2}$ (cf table 1 of LG or tables 4, 5 and 6 of I). The set of all inequivalent reps of \mathbf{L}^+ can be broken up into one-element and two-element classes (orbits) as follows. If $\bar{D}(\mathbf{L}^+) \sim \mathbf{D}(\mathbf{L}^+)$, the rep is self-conjugate (or of type 1). If two reps $\bar{D}(\mathbf{L}^+)$ and $\mathbf{D}(\mathbf{L}^+)$ are not equivalent, they are called mutually conjugate reps (or reps of type 2).

Now, if $\mathbf{D}(\mathbf{L}^+)$ is a self-conjugate rep, there exists a unitary matrix Z such that

$$\bar{D}(R^+|v+t) = Z^{-1}D(R^+|v+t)Z \quad (8)$$

for each element of \mathbf{L}^+ . In view of (6), the matrix Z can be chosen to be an involution (Herbut *et al* 1980):

$$Z^2 = I \quad (9)$$

where I is the unit matrix. The rep $\mathbf{D}(\mathbf{L}^+)$ then gives rise to two inequivalent reps $\mathbf{D}^\pm(\mathbf{L}^-)$ of \mathbf{L}^- defined by:

$$D^\pm(R^+|v+t) = D(R^+|v+t) \quad (10a)$$

$$D^\pm(R^-R^+|-v-t) = \pm ZD(R^+|v+t) \quad (10b)$$

(Herbut *et al* 1980), where $(R^-R^+|-v-t) = (R^-|0)(R^+|v+t)$. The reps $\mathbf{D}^\pm(\mathbf{L}^-)$ take over the quantum numbers of $\mathbf{D}(\mathbf{L}^+)$. For all the line groups, $\mathbf{D}(\mathbf{L}^+)$ is either one-dimensional or two-dimensional (cf I). In the first case,

$$Z = 1, \tag{11}$$

which was the only possibility found in I. If $\mathbf{D}(\mathbf{L}^+)$ is a two-dimensional rep, note first that, being unitary ($Z^\dagger = Z^{-1}$) and involutive ($Z = Z^{-1}$), Z is a Hermitian matrix, $Z^\dagger = Z$. Then only two possibilities exist. If $\bar{\mathbf{D}}(\mathbf{L}^+)$ is equal to $\mathbf{D}(\mathbf{L}^+)$ then Z is obviously trivial in view of (8):

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{12}$$

Otherwise, i.e. when $\bar{\mathbf{D}}(\mathbf{L}^+)$ and $\mathbf{D}(\mathbf{L}^+)$ are equivalent but not equal, Z is (since it is both Hermitian and unitary) of the form

$$Z = \begin{pmatrix} \sin \theta & \exp(i\phi)\cos \theta \\ \exp(-i\phi)\cos \theta & -\sin \theta \end{pmatrix} \tag{13}$$

where θ and ϕ are determined by (8).

If we have a conjugate pair of reps of \mathbf{L}^+ , $\mathbf{D}(\mathbf{L}^+)$ and $\bar{\mathbf{D}}(\mathbf{L}^+)$, they together induce one double-dimensional rep of \mathbf{L}^- , denoted by $\mathbf{Q}(\mathbf{L}^-)$:

$$Q(R^+|v+t) = \begin{pmatrix} D(R^+|v+t) & 0 \\ 0 & \bar{D}(R^+|v+t) \end{pmatrix} \tag{14a}$$

$$Q(R^-R^+|-v-t) = \begin{pmatrix} 0 & \bar{D}(R^+|v+t) \\ D(R^+|v+t) & 0 \end{pmatrix} \tag{14b}$$

(Herbut *et al* 1980). Obviously, $Q(R^-R^+|-v-t) = Q[(R^-|0)(R^+|v+t)] = Q(R^-|0)Q(R^+|v+t)$, where

$$Q(R^-|0) = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}. \tag{15}$$

The quantum numbers of both reps $\mathbf{D}(\mathbf{L}^+)$ and $\bar{\mathbf{D}}(\mathbf{L}^+)$ constitute together the label for $\mathbf{Q}(\mathbf{L}^-)$.

In conclusion, all the reps of the line groups isogonal to \mathbf{D}_{nd} or \mathbf{D}_{nh} , $n = 1, 2, 3, \dots$, can be constructed—either directly via (10a,b) or by induction (14a,b)—using the reps of the line groups \mathbf{L}^+ isogonal to \mathbf{C}_{nv} , $n = 1, 2, 3, \dots$. We therefore reproduce the latter reps (in tables 1, 2, 3 and 4) in a form suitable for our present purpose.

In the actual construction of the reps we also utilise the following useful facts proved in I.

(i) For $k = 0$ the reps of \mathbf{L}^- are the same as the reps of its isogonal point group (cf I (10)).

(ii) For $0 < k < \pi/a$ none of the reps of $\mathbf{D}(\mathbf{L}^+)$ is self-conjugate (cf (9) in I) and one uses only the induction procedure (14a, b).

(iii) For $k = \pi/a$ and if \mathbf{L}^- is symmorphic (i.e. $\mathbf{L}^- = \mathbf{T} \wedge \mathbf{P}$), the reps of \mathbf{L}^- are obtained by multiplying the reps of its isogonal point group by the factor $(-1)^l$.

Table 1. The reps of point groups C_{nv} , $n = 1, 2, 3, \dots$; $\alpha = 2\pi/n$, $s = 0, 1, \dots, n-1$; $m = 1, 2, \dots, \frac{1}{2}(n-1)$ if $n = 3, 5, 7, \dots$ and $m = 1, 2, \dots, \frac{1}{2}(n-2)$ if $n = 4, 6, 8, \dots$; $M(s) = \begin{pmatrix} \exp(ims\alpha) & 0 \\ 0 & \exp(-ims\alpha) \end{pmatrix}$, $P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Note that for $n=1$ and $n=2$ there are no two-dimensional reps.

Rep	C_n^s	$\sigma_v C_n^s$
A_0	1	1
B_0	1	-1
$E_{m,-m}$	$M(s)$	$PM(s)$
A_q^\dagger	$(-1)^s$	$(-1)^s$
B_q^\dagger	$(-1)^s$	$-(-1)^s$

† For $n = 2q = 2, 4, 6, \dots$ only.

Table 2. The reps of the line groups L_{nm} , $n = 1, 3, 5, \dots$ and L_{nmm} , $n = 2, 4, 6, \dots$. Here $-\pi/a < k \leq \pi/a$, $t = 0, \pm 1, \pm 2, \dots$ (or $t = 0, \pm 1, \pm 2, \dots, \pm N$ if the cyclic boundary condition $(E|2N+1) = (E|0)$ is assumed; cf I); for $\alpha, s, m, M(s)$ and P see the caption to table 1. In the cases of L_{1m} and L_{2mm} there are no two-dimensional reps.

Rep	$(C_n^s t)$	$(\sigma_v C_n^s t)$
${}_k A_0$	$\exp(ikta)$	$\exp(ikta)$
${}_k B_0$	$\exp(ikta)$	$-\exp(ikta)$
${}_k E_{m,-m}$	$\exp(ikta)M(s)$	$\exp(ikta)PM(s)$
${}_k A_q^\dagger$	$(-1)^s \exp(ikta)$	$(-1)^s \exp(ikta)$
${}_k B_q^\dagger$	$(-1)^s \exp(ikta)$	$-(-1)^s \exp(ikta)$

† For $n = 2q = 2, 4, 6, \dots$ only.

Table 3. The reps of the line groups L_{nc} , $n = 1, 3, 5, \dots$ and L_{ncc} , $n = 2, 4, 6, \dots$; $\alpha, s, m, M(s)$ and P as in table 1; t and k as in table 2. In the cases of L_{1c} and L_{2cc} there are no two-dimensional reps.

Rep	$(C_n^s t)$	$(\sigma_v C_n^s \frac{1}{2} + t)$
${}_k A_0$	$\exp(ikta)$	$\exp[ik(\frac{1}{2} + t)a]$
${}_k B_0$	$\exp(ikta)$	$-\exp[ik(\frac{1}{2} + t)a]$
${}_k E_{m,-m}$	$\exp(ikta)M(s)$	$\exp[ik(\frac{1}{2} + t)a]PM(s)$
${}_k A_q^\dagger$	$(-1)^s \exp(ikta)$	$(-1)^s \exp[ik(\frac{1}{2} + t)a]$
${}_k B_q^\dagger$	$(-1)^s \exp(ikta)$	$-(-1)^s \exp[ik(\frac{1}{2} + t)a]$

† For $n = 2q = 2, 4, 6, \dots$ only.

3. Construction of the reps of the line groups isogonal to D_{nd} , $n = 1, 2, 3, \dots$

3.1. Point groups D_{nd}

D_{nd} can be viewed as a semi-direct product of C_{nv} by $D'_1 = \{E, U_d\}$:

$$D_{nd} = C_{nv} \wedge D'_1 = C_{nv} + U_d C_{nv}. \tag{16}$$

Table 4. The reps of the line groups $\mathbf{L}(2q)_qmc$, $n = 2q = 2, 4, 6, \dots$; $\alpha, m, M(s)$ and P as in table 1; t and k as in table 2; $r = 0, 1, \dots, q - 1$. In the case of $\mathbf{L}2_1mc$ there are no two-dimensional reps.

Rep	$(C_{2q}^{2r} t)$	$(C_{2q}^{2r+1} \frac{1}{2}+t)$	$(\sigma_v C_{2q}^{2r} t)$	$(\sigma_v C_{2q}^{2r+1} \frac{1}{2}+t)$
${}_k A_0$	$\exp(ikta)$	$\exp[ik(\frac{1}{2}+t)a]$	$\exp(ikta)$	$\exp[ik(\frac{1}{2}+t)a]$
${}_k B_0$	$\exp(ikta)$	$\exp[ik(\frac{1}{2}+t)a]$	$-\exp(ikta)$	$-\exp[ik(\frac{1}{2}+t)a]$
${}_k E_{m,-m}$	$\exp(ikta)M(2r)$	$\exp[ik(\frac{1}{2}+t)a]M(2r+1)$	$\exp(ikta)PM(2r)$	$\exp[ik(\frac{1}{2}+t)a]PM(2r+1)$
${}_k A_q$	$\exp(ikta)$	$-\exp[ik(\frac{1}{2}+t)a]$	$\exp(ikta)$	$-\exp[ik(\frac{1}{2}+t)a]$
${}_k B_q$	$\exp(ikta)$	$-\exp[ik(\frac{1}{2}+t)a]$	$-\exp(ikta)$	$\exp[ik(\frac{1}{2}+t)a]$

The reps of \mathbf{D}_{nd} are constructed here by means of the reps of their invariant subgroups \mathbf{C}_{nv} (which are given in table 1) in the manner described in § 2.

3.1.1. Conjugate reps of \mathbf{C}_{nv} (cf table 1)

$$(a) \quad \bar{A}_0(C_n^s) = A_0(U_d C_n^s U_d^{-1}) = A_0(C_n^{-s}) = 1 = A_0(C_n^s)$$

$$\bar{A}_0(\sigma_v C_n^s) = A_0(U_d \sigma_v C_n^s U_d^{-1}) = A_0(\sigma_v C_n^{-s-1}) = 1 = A_0(\sigma_v C_n^s).$$

Therefore $\mathbf{A}_0(\mathbf{C}_{nv})$ is self-conjugate in \mathbf{D}_{nd} and thus it gives rise to two one-dimensional reps $\mathbf{A}_0^\pm(\mathbf{D}_{nd})$ as defined by (10a, b), with $Z = 1$, as in (11).

(b) In the same manner one shows that $\mathbf{B}_0(\mathbf{C}_{nv})$ is self-conjugate in \mathbf{D}_{nd} so that it produces two one-dimensional reps $\mathbf{B}_0^\pm(\mathbf{D}_{nd})$.

(c) Next

$$\bar{E}_{m,-m}(C_n^s) = E_{m,-m}(C_n^{-s}) = \begin{pmatrix} \exp(-ims\alpha) & 0 \\ 0 & \exp(ims\alpha) \end{pmatrix} = M(-s)$$

and

$$\bar{E}_{m,-m}(\sigma_v C_n^s) = E_{m,-m}(\sigma_v C_n^{-s-1}) = PM(-s-1),$$

where $M(s)$ and P are defined in the caption to table 1. But the reps $\mathbf{E}_{m,-m}(\mathbf{C}_{nv})$ and $\bar{\mathbf{E}}_{m,-m}(\mathbf{C}_{nv})$ are equivalent, since their characters are equal:

$$\text{Tr } M(s) = 2 \cos(ms\alpha) = \text{Tr } M(-s) \quad \text{Tr } PM(s) = 0 = \text{Tr } PM(-s-1).$$

In order to obtain $\mathbf{E}_{m,-m}^\pm(\mathbf{D}_{nd})$ by (10a, b) one needs the matrix Z of the form (13) and satisfying (8), which here amounts to

$$Z\bar{E}_{m,-m}(C_n^s) = E_{m,-m}(C_n^s)Z \tag{17a}$$

$$Z\bar{E}_{m,-m}(\sigma_v C_n^s) = E_{m,-m}(\sigma_v C_n^s)Z. \tag{17b}$$

Equation (17a) gives $\sin \theta = 0$ whereas (17b) requires $\exp(i\phi) = \exp(\frac{1}{2}im\alpha)$, so that

$$Z = \begin{pmatrix} 0 & \exp(\frac{1}{2}im\alpha) \\ \exp(-\frac{1}{2}im\alpha) & 0 \end{pmatrix} = PM(-\frac{1}{2}). \tag{18}$$

Therefore

$$E_{m,-m}^\pm(U_d C_n^s) = \pm PM(-\frac{1}{2})M(s) = PM(s - \frac{1}{2})$$

$$E_{m,-m}^\pm(U_d \sigma_v C_n^s) = \pm PM(-\frac{1}{2})PM(s) = \pm M(s + \frac{1}{2}) \quad \text{as } PM(\frac{1}{2})P = M(-\frac{1}{2}).$$

$$(d) \quad \begin{aligned} \bar{A}_q(C_n^s) &= A_q(C_n^{-s}) = (-1)^{-s} = B_q(C_n^s) \\ \bar{A}_q(\sigma_v C_n^s) &= A_q(\sigma_v C_n^{-s-1}) = (-1)^{-s-1} = B_q(\sigma C_n^s) \end{aligned}$$

so that $\mathbf{A}_q(\mathbf{C}_{nv})$ and $\mathbf{B}_q(\mathbf{C}_{nv})$ are mutually conjugate, thus giving rise to one two-dimensional rep as defined by (14a,b) which will be denoted as $\mathbf{E}_q(\mathbf{D}_{nd})$.

Table 5. The reps of point groups \mathbf{D}_{nd} , $n = 1, 2, 3, \dots$; for $\alpha, s, m, M(s)$ and P see the caption to table 1. Note that in the case of \mathbf{D}_{1d} there are no two-dimensional reps, while for \mathbf{D}_{2d} there is only one, $\mathbf{E}_1(\mathbf{D}_{2d})$.

Rep	C_n^s	$\sigma_v C_n^s$	$U_d C_n^s$	$U_d \sigma_v C_n^s$
A_0^\pm	1	1	± 1	± 1
B_0^\pm	1	-1	± 1	∓ 1
$E_{m,-m}^\pm$	$M(s)$	$PM(s)$	$\pm PM(s - \frac{1}{2})$	$\pm M(s + \frac{1}{2})$
E_q^\dagger	$(-1)^s \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$(-1)^s \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$(-1)^s \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$(-1)^s \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

† For $n = 2q = 2, 4, 6, \dots$ only.

3.2. Line groups $\mathbf{L}\bar{n}m$ and $\mathbf{L}(\bar{2}n)2m$

This is the first of the two families (i.e. the sets of line groups differing only in the order of the main axis) of line groups isogonal to \mathbf{D}_{nd} (cf LG). It consists of symmorphic line groups

$$\mathbf{L}\bar{n}m = \mathbf{L}nm + (U_d|0)\mathbf{L}nm \quad n = 1, 3, 5, \dots \tag{19a}$$

$$\mathbf{L}(\bar{2}n)2m = \mathbf{L}nmm + (U_d|0)\mathbf{L}nmm \quad n = 2, 4, 6, \dots \tag{19b}$$

whose elements are of the form $(C_n^s|t), (\sigma_v C_n^s|t), (U_d C_n^s|-t), (U_d \sigma C_n^s|-t)$. (Note that the latter two differ by the negative sign in front of t compared with the expressions given in LG; the above form is more convenient for our present purpose.)

3.2.1. Conjugate reps of $\mathbf{L}nm$ and $\mathbf{L}nmm$ (cf table 2)

(a) For $0 < k < \pi/a$ we have the conjugate pairs of reps

$$\begin{aligned} {}_k\bar{A}_0(C_n^s|t) &= {}_kA_0[(U_d|0)(C_n^s|t)(U_d|0)^{-1}] \\ &= {}_kA_0(U_d C_n^s U_d^{-1}|-t) = {}_kA_0(C_n^{-s}|-t) \\ &= \exp(-ikta) = -{}_kA_0(C_n^s|t) \end{aligned}$$

and

$${}_k\bar{A}_0(\sigma_v C_n^s|t) = {}_kA_0(\sigma_v C_n^{-s-1}|-t) = \exp(-ikta) = -{}_kA_0(\sigma_v C_n^s|t).$$

Thus ${}_k\mathbf{A}_0(\mathbf{L}nm)$ and $-{}_k\mathbf{A}_0(\mathbf{L}nm)$ together give rise to the induced two-dimensional rep of $\mathbf{L}\bar{n}m$, which we denote by ${}^{-k}_k\mathbf{E}_{A_0}(\mathbf{L}\bar{n}m)$, $n = 1, 3, 5, \dots$

(b) Analogously, ${}_k\bar{B}_0(C_n^s|t) = \exp(-ikta) = -{}_kB_0(C_n^s|t)$ and ${}_k\bar{B}_0(\sigma_v C_n^s|t) = -\exp(-ikta) = -{}_kB_0(\sigma_v C_n^s|t)$, inducing ${}^{-k}_k\mathbf{E}_{B_0}(\mathbf{L}\bar{n}m)$, $n = 1, 3, 5, \dots$

(c) Next

$${}_k\bar{E}_{m,-m}(C_n^s | t) = {}_kE_{m,-m}(C_n^{-s} | -t) = \exp(-ikta)M(-s)$$

and

$${}_k\bar{E}_{m,-m}(\sigma_v C_n^s | t) = {}_kE_{m,-m}(\sigma_v C_n^{-s-1} | -t) = \exp(-ikta)PM(-s-1).$$

Comparing the characters of ${}_{-k}\mathbf{E}_{m,-m}(\mathbf{L}nm)$ and ${}_k\bar{\mathbf{E}}_{m,-m}(\mathbf{L}nm)$ one finds that they are equivalent; hence ${}_k\mathbf{E}_{m,-m}$ and ${}_{-k}\mathbf{E}_{m,-m}$ induce a four-dimensional rep, ${}_{-k}^k\mathbf{G}_{m,-m}(\mathbf{L}\bar{n}m)$, $n = 3, 5, 7, \dots$

All that is said in (a), (b) and (c) applies also to $\mathbf{L}(\bar{2n})2m$, $n = 2, 4, 6, \dots$. Thus we have ${}_{-k}^k\mathbf{E}_{A_0}(\mathbf{L}(\bar{2n})2m)$, ${}_{-k}^k\mathbf{E}_{B_0}(\mathbf{L}(\bar{2n})2m)$, $n = 2, 4, 6, \dots$ and ${}_{-k}^k\mathbf{G}_{m,-m}(\mathbf{L}(\bar{2n})2m)$, $n = 4, 6, 8, \dots$. In addition, for $n = 2, 4, 6, \dots$, we have

$$(d) \quad {}_k\bar{A}_q(C_n^s | t) = {}_kA_q(C_n^{-s} | -t) = (-1)^{-s} \exp(-ikta) = {}_{-k}B_q(C_n^s | t)$$

$${}_k\bar{A}_q(\sigma_v C_n^s | t) = {}_kA_q(\sigma_v C_n^{-s-1} | -t) = (-1)^{-s-1} \exp(-ikta) = {}_{-k}B_q(\sigma_v C_n^s | t),$$

giving rise to ${}_{-k}^k\mathbf{E}_{A_q}^B(\mathbf{L}(\bar{2n})2m)$.

(e) Analogously, ${}_k\bar{B}_q(C_n^s | t) = {}_{-k}A_q(C_n^s | t)$ and ${}_k\bar{B}_q(\sigma_v C_n^s | t) = {}_{-k}A_q(\sigma_v C_n^s | t)$, which gives ${}_{-k}^k\mathbf{E}_{B_q}^A(\mathbf{L}(\bar{2n})2m)$.

The line groups considered are symmorphoric and their reps at $k = \pi/a$ are obtained by multiplying those of \mathbf{D}_{nd} (cf table 5) by $(-1)^t$.

3.3. Line groups $\mathbf{L}\bar{n}c$ and $\mathbf{L}(\bar{2n})2c$

The second family of line groups isogonal to \mathbf{D}_{nd} consists of non-symmorphoric line groups (cf LG):

$$\mathbf{L}\bar{n}c = \mathbf{L}nc + (U_d | 0)\mathbf{L}nc \quad n = 1, 3, 5, \dots \tag{20a}$$

$$\mathbf{L}(\bar{2n})2c = \mathbf{L}ncc + (U_d | 0)\mathbf{L}ncc \quad n = 2, 4, 6, \dots \tag{20b}$$

whose elements are of the form $(C_n^s | t)$, $(\sigma_v C_n^s | \frac{1}{2} + t)$, $(U_d C_n^s | -t)$, $(U_d \sigma_v C_n^s | -\frac{1}{2} - t)$. (The latter two differ by the negative sign in front of translations from those given in LG.)

3.3.1. Conjugate reps of $\mathbf{L}nc$ and $\mathbf{L}ncc$ (cf table 3)

(a) for $0 < k < \pi/a$ one has

$${}_k\bar{A}_0(C_n^s | t) = {}_kA_0(C_n^{-s} | -t) = \exp(-ikta) = {}_{-k}A_0(C_n^s | t)$$

and

$${}_k\bar{A}_0(\sigma_v C_n^s | \frac{1}{2} + t) = {}_kA_0(\sigma_v C_n^{-s-1} | -\frac{1}{2} - t) = \exp[-ik(\frac{1}{2} + t)a] = {}_{-k}A_0(\sigma_v C_n^s | \frac{1}{2} + t)$$

so that ${}_k\mathbf{A}_0$ and ${}_{-k}\mathbf{A}_0$ induce a two-dimensional rep, ${}_{-k}^k\mathbf{E}_{A_0}$.

(b) Similarly, ${}_k\mathbf{B}_0$ and ${}_{-k}\mathbf{B}_0$ induce ${}_{-k}^k\mathbf{E}_{B_0}$.

(c) Next

$${}_k\bar{E}_{m,-m}(C_n^s | t) = {}_kE_{m,-m}(C_n^{-s} | -t) = \exp(-ikta)M(-s)$$

$${}_k\bar{E}_{m,-m}(\sigma_v C_n^s | \frac{1}{2} + t) = {}_kE_{m,-m}(\sigma_v C_n^{-s-1} | -\frac{1}{2} - t) = \exp[-ik(\frac{1}{2} + t)a]PM(-s-1).$$

Comparing the characters one finds that ${}_k\bar{\mathbf{E}}_{m,-m} \sim {}_{-k}\mathbf{E}_{m,-m}$, so that ${}_k\mathbf{E}_{m,-m}$ and ${}_{-k}\mathbf{E}_{m,-m}$ induce a four-dimensional rep ${}_{-k}^k\mathbf{G}_{m,-m}$.

Table 6. The reps of the line groups $\mathbf{L}\bar{n}m$, $n = 1, 3, 5, \dots$ and $\mathbf{L}(\overline{2n})2m$, $n = 2, 4, 6, \dots$; α, s , $M(s)$ and P as in table 1; t as in table 2; $0 < k < \pi/a$;

$$K(t) = \begin{pmatrix} \exp(ikta) & 0 \\ 0 & \exp(-ikta) \end{pmatrix} \quad K'(t) = \begin{pmatrix} \exp(ikta) & 0 \\ 0 & -\exp(-ikta) \end{pmatrix}.$$

For $k = 0$ the reps of these line groups coincide with those of \mathbf{D}_{nd} and can be found in table 5. Thus, ${}^0\mathbf{A}_0$ ($\mathbf{L}\bar{n}m$) = $\mathbf{A}_0(\mathbf{D}_{nd})$, etc. Note that $\mathbf{L}\bar{1}m$ ($n = 1$) and $\mathbf{L}\bar{4}2m$ ($n = 2$) have neither ${}^{-k}\mathbf{G}_{m,-m}$ nor ${}_{\pi/a}\mathbf{E}_{m,-m}^\pm$ reps.

Reps	$(C_n^s t)$	$(\sigma_v C_n^s t)$
${}^{-k}E_{A_0}$	$K(t)$	$K(t)$
${}^{-k}E_{B_0}$	$K(t)$	$-K(t)$
${}^{-k}G_{m,-m}$	$\begin{pmatrix} \exp(ikta)M(s) & 0 \\ 0 & \exp(-ikta)M(-s) \end{pmatrix}$	$\begin{pmatrix} \exp(ikta)PM(s) & 0 \\ 0 & \exp(-ikta)PM(-s-1) \end{pmatrix}$
${}_{\pi/a}A_0^\pm$	$(-1)^t$	$(-1)^t$
${}_{\pi/a}B_0^\pm$	$(-1)^t$	$-(-1)^t$
${}_{\pi/a}E_{m,-m}^\pm$	$(-1)^t M(s)$	$(-1)^t PM(s)$
${}^{-k}E_{A_q}^{B_q \dagger}$	$(-1)^s K(t)$	$(-1)^s K'(t)$
${}^{-k}E_{B_q}^{A_q \dagger}$	$(-1)^s K(t)$	$-(-1)^s K'(t)$
${}_{\pi/a}E_q^\dagger$	$(-1)^{s+t} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$(-1)^{s+t} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Rep	$(U_d C_n^s -t)$	$(U_d \sigma_v C_n^s -t)$
${}^{-k}E_{A_0}$	$PK(t)$	$PK(t)$
${}^{-k}E_{B_0}$	$PK(t)$	$-PK(t)$
${}^{-k}G_{m,-m}$	$\begin{pmatrix} 0 & \exp(-ikta)M(-s) \\ \exp(ikta)M(s) & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \exp(-ikta)PM(-s-1) \\ \exp(ikta)PM(s) & 0 \end{pmatrix}$
${}_{\pi/a}A_0^\pm$	$\pm(-1)^t$	$\pm(-1)^t$
${}_{\pi/a}B_0^\pm$	$\pm(-1)^t$	$\mp(-1)^t$
${}_{\pi/a}E_{m,-m}^\pm$	$\pm(-1)^t PM(s - \frac{1}{2})$	$\pm(-1)^t M(s + \frac{1}{2})$
${}^{-k}E_{A_q}^{B_q \dagger}$	$(-1)^s PK(t)$	$(-1)^s PK'(t)$
${}^{-k}E_{B_q}^{A_q \dagger}$	$(-1)^s PK(t)$	$-(-1)^s PK'(t)$
${}_{\pi/a}E_q^\dagger$	$(-1)^{s+t} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$(-1)^{s+t} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

† For $n = 2q = 2, 4, 6, \dots$ only.

Finally, in the case when $n = 2q = 2, 4, 6, \dots$, one also has

$$\begin{aligned} (d) \quad {}_k\bar{A}_q(C_n^s | t) &= {}_kA_q(C_n^{-s} | -t) = (-1)^{-2} \exp(-ikta) = -{}_kB_q(C_n^s | t) \\ {}_k\bar{A}_q(\sigma_v C_n^s | \frac{1}{2} + t) &= {}_kA_q(\sigma_v C_n^{-s} | -\frac{1}{2} - t) = (-1)^{-s-1} \exp[-ik(\frac{1}{2} + t)a] \\ &= -{}_kB_q(\sigma_v C_n^s | \frac{1}{2} + t), \end{aligned}$$

giving rise to ${}^{-k}E_{A_q}^{B_q}(\mathbf{L}(\overline{2n})2c)$.

(e) Similarly, ${}_k\bar{B}_q = -{}_kA_q$, so that one induces ${}^{-k}E_{B_q}^{A_q}(\mathbf{L}(\overline{2n})2c)$.

Since the groups we are considering now are non-symmorphic ones, a similar analysis of conjugate reps is required for $k = \pi/a$.

$$(f) \quad \begin{aligned} \pi/a \bar{A}_0(C_n^s | t) &= (-1)^{-t} = \pi/a B_0(C_n^s | t) \\ \pi/a \bar{A}_0(\sigma_v C_n^s | \frac{1}{2} + t) &= -i(-1)^t = \pi/a B_0(\sigma_v C_n^s | \frac{1}{2} + t) \end{aligned}$$

so that we obtain $\pi/a \mathbf{E}_0$.

(g) Next, $\pi/a \bar{E}_{m,-m}(C_n^s | t) = (-1)^t M(-s)$ and $\pi/a \bar{E}_{m,-m}(\sigma_v C_n^s | \frac{1}{2} + t) = -i(-1)^t PM(-s-1)$. Thus $\pi/a \bar{E}_{m,-m} \sim \pi/a \mathbf{E}_{m,-m}$, i.e. it is self-conjugate and gives rise to two reps $\pi/a \mathbf{E}_{m,-m}^\pm$ as defined by (10a,b), where the matrix z is found according to (8) to be

$$Z = \begin{pmatrix} 0 & i \exp(\frac{1}{2}i m \alpha) \\ -i \exp(-\frac{1}{2}i m \alpha) & 0 \end{pmatrix} = -i PM'(-\frac{1}{2}).$$

Again, for $n = 2q = 2, 4, 6, \dots$, one has some additional reps:

$$(h) \quad \pi/a \bar{A}_q(C_n^s | t) = (-1)^{-s-t} = \pi/a A_q(C_n^s | t)$$

Table 7. The reps of the line groups $L\bar{n}c, n = 1, 3, 5, \dots$ and $L(\overline{2n})2c, n = 2, 4, 6, \dots$; $\alpha, s, m, M(s)$ and P as in table 1; t as in table 2; $k, K(t)$ and $K'(t)$ as in table 6;

$$M'(s) = \begin{pmatrix} \exp(ims\alpha) & 0 \\ 0 & -\exp(-ims\alpha) \end{pmatrix}.$$

For $k = 0$ reps see the remark in the caption to table 6. Note that $L\bar{1}c$ and $L\bar{4}2c$ have neither ${}^{-k}G_{m,-m}$ nor $\pi/a \mathbf{E}_{m,-m}^\pm$ reps.

Rep	$(C_n^s t)$	$(\sigma_v C_n^s \frac{1}{2} + t)$
${}^{-k}E_{A_0}$	$K(t)$	$K(\frac{1}{2} + t)$
${}^{-k}E_{B_0}$	$K(t)$	$-K(\frac{1}{2} + t)$
${}^{-k}G_{m,-m}$	$\begin{pmatrix} \exp(ikta)M(s) & 0 \\ 0 & \exp(-ikta)M(-s) \end{pmatrix}$	$\begin{pmatrix} \exp[ik(\frac{1}{2} + t)a]PM(s) & 0 \\ 0 & \exp[-ik(\frac{1}{2} + t)a]PM(-s-1) \end{pmatrix}$
$\pi/a E_0$	$(-1)^t \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$(-1)^t \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix}$
$\pi/a E_{m,-m}^\pm$	$(-1)^t M(s)$	$i(-1)^t PM(s)$
${}^{-k}E_{A_q}^\dagger$	$(-1)^s K(t)$	$(-1)^s K'(\frac{1}{2} + t)$
${}^{-k}E_{B_q}^\dagger$	$(-1)^s K(t)$	$-(-1)^s K'(\frac{1}{2} + t)$
$\pi/a A_q^\dagger$	$(-1)^{s+t}$	$i(-1)^{s+t}$
$\pi/a B_q^\dagger$	$(-1)^{s+t}$	$-i(-1)^{s+t}$
Rep	$(U_d C_n^s -t)$	$(U_d \sigma_v C_n^s -\frac{1}{2} - t)$
${}^{-k}E_{A_0}$	$PK(t)$	$PK(\frac{1}{2} + t)$
${}^{-k}E_{B_0}$	$PK(t)$	$-PK(\frac{1}{2} + t)$
${}^{-k}G_{m,-m}$	$\begin{pmatrix} 0 & \exp(-ikta)M(-s) \\ \exp(ikta)M(s) & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \exp[-ik(\frac{1}{2} + t)a]PM(-s-1) \\ \exp[ik(\frac{1}{2} + t)a]PM(s) & 0 \end{pmatrix}$
$\pi/a E_0$	$(-1)^t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$(-1)^t \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
$\pi/a E_{m,-m}^\pm$	$\pm i(-1)^t PM'(s - \frac{1}{2})$	$\mp(-1)^t M'(s + \frac{1}{2})$
${}^{-k}E_{A_q}^\dagger$	$(-1)^s PK(t)$	$(-1)^s PK'(\frac{1}{2} + t)$
${}^{-k}E_{B_q}^\dagger$	$(-1)^s PK(t)$	$-(-1)^s PK'(\frac{1}{2} + t)$
$\pi/a A_q^\dagger$	$\pm(-1)^{s+t}$	$\pm i(-1)^{s+t}$
$\pi/a B_q^\dagger$	$\pm(-1)^{s+t}$	$\mp i(-1)^{s+t}$

† For $n = 2q = 2, 4, 6, \dots$ only.

and

$$\pi/a \bar{A}_q(\sigma_v C_n^s | \frac{1}{2} + t) = -i(-1)^{-s-1-t} = \pi/a A_q(\sigma_v C_n^s | \frac{1}{2} + t)$$

so that one has $\pi/a \mathbf{A}_q^\pm(\mathbf{L}(\overline{2n})2c)$, where $Z = 1$ as in (11).

(i) Similarly one finds that $\pi/a \bar{\mathbf{B}}_q = \pi/a \mathbf{B}_q$, giving rise to $\pi/a \mathbf{B}_q^\pm(\mathbf{L}(\overline{2n})2c)$, also with $Z = 1$.

4. Construction of the reps of the line groups isogonal to \mathbf{D}_{nh} , $n = 1, 2, 3, \dots$

4.1. Point groups \mathbf{D}_{nh}

\mathbf{D}_{nh} is a direct product of \mathbf{C}_{nv} and $\mathbf{C}_{1h} = \{E, \sigma_h\}$:

$$\mathbf{D}_{nh} = \mathbf{C}_{nv} \otimes \mathbf{C}_{1h} = \mathbf{C}_{nv} + \sigma_h \mathbf{C}_{nv}, \tag{21}$$

which implies $\sigma_h C_h^s \sigma_h^{-1} = C_h^s$ and $\sigma_h \sigma_v C_n^s \sigma_h^{-1} = \sigma_v C_n^s$, so that every rep of \mathbf{C}_{nv} is equal to its rep conjugate by σ_h in \mathbf{D}_{nh} . Thus all the reps of \mathbf{D}_{nh} are obtained from those of \mathbf{C}_{nv} (which are given in table 1) directly via (10a,b) with Z trivial.

Table 8. The reps of point groups \mathbf{D}_{nh} , $n = 1, 2, 3, \dots$. For $\alpha, s, m, M(s)$ and P see the caption to table 1. Note that in the case of \mathbf{D}_{1h} and \mathbf{D}_{2h} there are no two-dimensional reps.

Rep	C_n^s	$\sigma_v C_n^s$	$\sigma_h C_n^s$	$\sigma_h \sigma_v C_n^s$
A_0^\pm	1	1	± 1	± 1
B_0^\pm	1	-1	± 1	∓ 1
$E_{m,-m}^\pm$	$M(s)$	$PM(s)$	$\pm M(s)$	$\pm PM(s)$
$A_q^{\pm \dagger}$	$(-1)^s$	$(-1)^s$	$\pm (-1)^s$	$\pm (-1)^s$
$B_q^{\pm \dagger}$	$(-1)^s$	$-(-1)^s$	$\pm (-1)^s$	$\mp (-1)^s$

\dagger For $n = 2q = 2, 4, 6, \dots$ only.

4.2. Line groups $\mathbf{L}(\overline{2n})2m$ and \mathbf{Ln}/mmm

This is the first family of line groups isogonal to \mathbf{D}_{nh} . The family consists of symmorphic line groups (cf LG):

$$\mathbf{L}(\overline{2n})2m = \mathbf{Lnm} + (\sigma_h | 0) \mathbf{Lnm} \quad n = 1, 3, 5, \dots \tag{22a}$$

$$\mathbf{Ln}/mmm = \mathbf{Lnmm} + (\sigma_h | 0) \mathbf{Lnmm} \quad n = 2, 4, 6, \dots \tag{22b}$$

with elements of the form $(C_n^s | t), (\sigma_v C_n^s | t), (\sigma_h C_n^s | -t), (\sigma_h \sigma_v C_n^s | -t)$. (Compared with LG, there is a change $t \rightarrow -t$ in the latter two.)

4.2.1. Conjugate reps of \mathbf{Lnm} and \mathbf{Lnmm} (cf table 2). Since

$$(\sigma_h | 0)(C_n^s | t)(\sigma_h | 0)^{-1} = (C_n^s | -t)$$

and

$$(\sigma_h | 0)(\sigma_v C_n^s | t)(\sigma_h | 0)^{-1} = (\sigma_v C_n^s | -t),$$

one easily finds reps of \mathbf{Lnm} and \mathbf{Lnmm} conjugate by $(\sigma_h | 0)$ in $\mathbf{L}(\overline{2n})2m$ and \mathbf{Ln}/mmm , respectively. Namely, the reps of \mathbf{Lnm} and \mathbf{Lnmm} are of the form (cf tables 1

and 2) ${}_k D_m(R|t) = \exp(ikta)D_m(R)$, so that here ${}_k \bar{D}_m(R|t) = {}_k D_m(R|-t) = \exp(-ikta)D_m(R) = -{}_k D_m(R|t)$. Hence for $0 < k < \pi/a$ we have conjugate pairs of reps of $\mathbf{Ln}m$ (and $\mathbf{Ln}mm$) with opposite k , which induce via (14a,b) reps of $\mathbf{L}(\bar{2}n)2m$ (and \mathbf{Ln}/mmm). As the line groups considered are symmorphic, their $k = \pi/a$ reps are obtained by multiplying those of \mathbf{D}_{nh} (cf table 8) by $(-1)^t$.

Table 9. The reps of the line groups $\mathbf{L}(\bar{2}n)2m, n = 1, 3, 5, \dots$ and $\mathbf{Ln}/mmm, n = 2, 4, 6, \dots$. For $\alpha, s, m, M(s)$ and P see table 1, for t see table 2 and for $k, K(t)$ see table 6. For $k = 0$ the reps of the line groups considered coincide with those of \mathbf{D}_{nh} , which are given in table 8; thus one has ${}_0 \mathbf{A}_0(\mathbf{L}(\bar{2}n)2m) = \mathbf{A}_0(\mathbf{D}_{nh})$, etc. Note that $\mathbf{L}\bar{2}2m$ (i.e. for $n = 1$) and $\mathbf{L}2/mmm$ (i.e. for $n = 2$) have neither ${}^{-k} \mathbf{G}_{m,-m}$ nor ${}_{\pi/a} \mathbf{E}_{m,-m}^\pm$ reps.

Rep	$(C_n^s t)$	$(\sigma_v C_n^s t)$
${}^{-k} E_{A_0}$	$K(t)$	$K(t)$
${}^{-k} E_{B_0}$	$K(t)$	$-K(t)$
${}^{-k} G_{m,-m}$	$\begin{pmatrix} \exp(ikta)M(s) & 0 \\ 0 & \exp(-ikta)M(s) \end{pmatrix}$	$\begin{pmatrix} \exp(ikta)PM(s) & 0 \\ 0 & \exp(-ikta)PM(s) \end{pmatrix}$
${}_{\pi/a} A_0^\pm$	$(-1)^t$	$(-1)^t$
${}_{\pi/a} B_0^\pm$	$(-1)^t$	$-(-1)^t$
${}_{\pi/a} E_{m,-m}^\pm$	$(-1)^t M(s)$	$(-1)^t PM(s)$
${}^{-k} E_{A_q}^\dagger$	$(-1)^s K(t)$	$(-1)^s K(t)$
${}^{-k} E_{B_q}^\dagger$	$(-1)^s K(t)$	$-(-1)^s K(t)$
${}_{\pi/a} A_q^\pm$	$(-1)^{s+t}$	$(-1)^{s+t}$
${}_{\pi/a} B_q^\pm$	$(-1)^{s+t}$	$-(-1)^{s+t}$

Rep	$(\sigma_h C_n^s -t)$	$(\sigma_h \sigma_v C_n^s -t)$
${}^{-k} E_{A_0}$	$PK(t)$	$PK(t)$
${}^{-k} E_{B_0}$	$PK(t)$	$-PK(t)$
${}^{-k} G_{m,-m}$	$\begin{pmatrix} 0 & \exp(-ikta)M(s) \\ \exp(ikta)M(s) & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \exp(-ikta)PM(s) \\ \exp(ikta)PM(s) & 0 \end{pmatrix}$
${}_{\pi/a} A_0^\pm$	$\pm(-1)^t$	$\pm(-1)^t$
${}_{\pi/a} B_0^\pm$	$\pm(-1)^t$	$\mp(-1)^t$
${}_{\pi/a} E_{m,-m}^\pm$	$\pm(-1)^t M(s)$	$\pm(-1)^t PM(s)$
${}^{-k} E_{A_q}^\dagger$	$(-1)^s PK(t)$	$(-1)^s PK(t)$
${}^{-k} E_{B_q}^\dagger$	$(-1)^s PK(t)$	$-(-1)^s PK(t)$
${}_{\pi/a} A_q^\pm$	$\pm(-1)^{s+t}$	$\pm(-1)^{s+t}$
${}_{\pi/a} B_q^\pm$	$\pm(-1)^{s+t}$	$\mp(-1)^{s+t}$

† For $n = 2q = 2, 4, 6, \dots$ only.

4.3. Line groups $\mathbf{L}(\bar{2}n)2c$ and \mathbf{Ln}/mcc

This family consists of non-symmorphic line groups which contain glide planes:

$$\mathbf{L}(\bar{2}n)2c = \mathbf{L}nc + (\sigma_h|0)\mathbf{L}nc \quad n = 1, 3, 5, \dots \tag{23a}$$

$$\mathbf{Ln}/mcc = \mathbf{L}ncc + (\sigma_h|0)\mathbf{L}ncc \quad n = 2, 4, 6, \dots \tag{23b}$$

Their elements are of the form $(C_n^s|t), (\sigma_v C_n^s|\frac{1}{2}+t), (\sigma_h C_n^s|-t), (\sigma_h \sigma_v C_n^s|-\frac{1}{2}-t)$. (Note the change of the sign of translations in the latter two elements as compared with that

found in LG. Also, it seems preferable to write \mathbf{Ln}/mcc , since every vertical plane here is a glide plane.)

4.3.1. *Conjugate reps of \mathbf{Lnc} and \mathbf{Lncc} (cf table 3)*

(a) For $0 < k < \pi/a$, the discussion is quite analogous to that given in § 4.2.1.

(b) However, for $k = \pi/a$ one has to examine each rep of \mathbf{Lnm} and \mathbf{Lnmm} . Thus $\pi/a \bar{\mathbf{A}}_0(C_n^s | t) = \pi/a \mathbf{A}_0(C_n^s | -t) = (-1)^{-t} = \pi/a \mathbf{B}_0(C_n^s | t)$, and $\pi/a \bar{\mathbf{A}}_0(\sigma_v C_n^s | \frac{1}{2} + t) = \pi/a \mathbf{A}_0(\sigma_v C_n^s | -\frac{1}{2} - t) = -i(-1)^{-t} = \pi/a \mathbf{B}_0(\sigma_v C_n^s | \frac{1}{2} + t)$, thus giving rise to $\pi/a \mathbf{E}_0$.

(c)
$$\pi/a \bar{\mathbf{E}}_{m,-m}(C_n^s | t) = (-1)^{-t} M(s)$$

and

$$\pi/a \bar{\mathbf{E}}_{m,-m}(\sigma_v C_n^s | \frac{1}{2} + t) = -i(-1)^{-t} PM(s),$$

so that the character is the same as before conjugation; hence $\pi/a \mathbf{E}_{m,-m} \sim \pi/a \bar{\mathbf{E}}_{m,-m}$. The matrix Z is of the form (13) and has to satisfy (8), which here specialises into

$$ZM(s) = M(s)Z$$

and

$$-ZPM(s) = PM(s)Z,$$

which gives

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{24}$$

so that $ZM(s) = M'(s)$.

(d) As in (a), one finds that $\pi/a \bar{\mathbf{A}}_q = \pi/a \mathbf{B}_q$, thus inducing $\pi/a \mathbf{E}_q$.

4.4. *Line groups $\mathbf{L}(2q)_q/mcm$*

The last family of line groups isogonal to \mathbf{D}_{nh} consists of non-symmorphic groups:

$$\mathbf{L}(2q)_q/mcm = \mathbf{L}(2q)_qmc + (\sigma_h | 0)\mathbf{L}(2q)_qmc \quad q = 1, 2, 3, \dots \tag{25}$$

Their elements are of the form $(C_{2q}^{2r} | t)$, $(C_{2q}^{2r+1} | \frac{1}{2} + t)$, $(\sigma_v C_{2q}^{2r} | t)$, $(\sigma_v C_{2q}^{2r+1} | \frac{1}{2} + t)$, $(\sigma_h C_{2q}^{2r} | -t)$, $(\sigma_h C_{2q}^{2r+1} | -\frac{1}{2} - t)$, $(\sigma_h \sigma_v C_{2q}^{2r} | -t)$, $(\sigma_h \sigma_v C_{2q}^{2r+1} | -\frac{1}{2} - t)$, where $r = 0, 1, \dots, q-1$. (In LG the translations have a positive sign. All indices $2r$ were misprinted there as $2r$.)

4.4.1. *Conjugate reps of $\mathbf{L}(2q)_qmc$ (cf table 4)*

(a) For $0 < k < \pi/a$ conjugate pairs of reps of $\mathbf{L}(2q)_qmc$ (with opposite values of k) induce via (14a,b) reps of $\mathbf{L}(2q)_q/mcm$; the argument is quite analogous to that of § 4.2.1.

(b) For $k = \pi/a$ we have

$$\begin{aligned} \pi/a \bar{\mathbf{A}}_0(C_{2q}^{2r} | t) &= \pi/a \bar{\mathbf{A}}_0(\sigma_v C_{2q}^{2r} | t) = (-1)^{-t} = \pi/a \mathbf{A}_q(C_{2q}^{2r} | t) = \pi/a \mathbf{A}_q(\sigma_v C_{2q}^{2r} | t) \\ \pi/a \bar{\mathbf{A}}_0(C_{2q}^{2r+1} | \frac{1}{2} + t) &= \pi/a \bar{\mathbf{A}}_0(\sigma_v C_{2q}^{2r+1} | \frac{1}{2} + t) = -i(-1)^{-t} = \pi/a \mathbf{A}_q(C_{2q}^{2r+1} | \frac{1}{2} + t) \\ &= \pi/a \mathbf{A}_q(\sigma_v C_{2q}^{2r+1} | \frac{1}{2} + t), \end{aligned}$$

thus inducing a two-dimensional rep, $\pi/a \mathbf{E}_{A_0^A}$.

Table 10. The reps of the line groups $L(\overline{2n})2c$, $n = 1, 3, 5, \dots$ and Ln/mcc , $n = 2, 4, 6, \dots$. For $\alpha, s, m, M(s)$ and P see table 1, for t see table 2, for $k, K(t)$ see table 6 and for $M'(s)$ see table 7. For $k = 0$ reps see the comment in the caption to table 9. Note that $L\overline{2}2c$ and $L\overline{2}/mcc$ have neither ${}^{-k}G_{m,-m}$ nor ${}_{\pi/a}E_{m,-m}^{\pm}$ reps.

Rep	$(C_n^s t)$	$(\sigma_v C_n^s \frac{1}{2} + t)$
${}^{-k}E_{A_0}$	$K(t)$	$K(\frac{1}{2} + t)$
${}^{-k}E_{B_0}$	$K(t)$	$-K(\frac{1}{2} + t)$
${}^{-k}G_{m,-m}$	$\begin{pmatrix} \exp(ikta)M(s) & 0 \\ 0 & \exp(-ikta)M(s) \end{pmatrix}$	$\begin{pmatrix} \exp[ik(\frac{1}{2} + t)a]PM(s) & 0 \\ 0 & \exp[-ik(\frac{1}{2} + t)a]PM(s) \end{pmatrix}$
${}_{\pi/a}E_0$	$(-1)^t \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$(-1)^t \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$
${}_{\pi/a}E_{m,-m}^{\pm}$	$(-1)^t M(s)$	$i(-1)^t PM(s)$
${}^{-k}E_{A_q}^{\dagger}$	$(-1)^s K(t)$	$(-1)^s K(\frac{1}{2} + t)$
${}^{-k}E_{B_q}^{\dagger}$	$(-1)^s K(t)$	$-(-1)^s K(\frac{1}{2} + t)$
${}_{\pi/a}E_{q}^{\dagger}$	$(-1)^{s+t} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$(-1)^{s+t} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$

Rep	$(\sigma_h C_n^s -t)$	$(\sigma_h \sigma_v C_n^s -\frac{1}{2} - t)$
${}^{-k}E_{A_0}$	$PK(t)$	$PK(\frac{1}{2} + t)$
${}^{-k}E_{B_0}$	$PK(t)$	$-PK(\frac{1}{2} + t)$
${}^{-k}G_{m,-m}$	$\begin{pmatrix} 0 & \exp(-ikta)M(s) \\ \exp(ikta)M(s) & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \exp[-ik(\frac{1}{2} + t)a]PM(s) \\ \exp[ik(\frac{1}{2} + t)a]PM(s) & 0 \end{pmatrix}$
${}_{\pi/a}E_0$	$(-1)^t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$(-1)^t \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
${}_{\pi/a}E_{m,-m}^{\pm}$	$\pm(-1)^t M'(s)$	$\mp i(-1)^t PM'(s)$
${}^{-k}E_{A_q}^{\dagger}$	$(-1)^s PK(t)$	$(-1)^s PK(\frac{1}{2} + t)$
${}^{-k}E_{B_q}^{\dagger}$	$(-1)^s PK(t)$	$-(-1)^s PK(\frac{1}{2} + t)$
${}_{\pi/a}E_{q}^{\dagger}$	$(-1)^{s+t} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$(-1)^{s+t} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

+ For $n = 2q = 2, 4, 6, \dots$ only.

(c) Similarly, ${}_{\pi/a}\bar{B}_0 = {}_{\pi/a}B_q$, giving together ${}_{\pi/a}E_{B_0}^B$.

(d) ${}_{\pi/a}\bar{E}_{m,-m}(C_{2q}^{2r} | t) = (-1)^{-t} M(2r)$

and

$${}_{\pi/a}\bar{E}_{m,-m}(C_{2q}^{2r+1} | \frac{1}{2} + t) = -i(-1)^{-t} M(2r + 1),$$

while the other matrices of ${}_{\pi/a}E_{m,-m}(L(2q)_q/mc)$ have trace equal to zero and need not be considered in what follows. To find m' such that ${}_{\pi/a}\bar{E}_{m,-m} \sim {}_{\pi/a}E_{m',-m'}$ one has to equal their characters:

$$\begin{aligned} (-1)^t 2 \cos(2rm\alpha) &= (-1)^t 2 \cos(2rm'\alpha) \\ -i(-1)^t \cos[(2r + 1)m\alpha] &= i(-1)^t 2 \cos[(2r + 1)m'\alpha] \end{aligned}$$

where $m, m' = 1, 2, \dots, q - 1$ (cf the caption to table 1); the solution is $m' = q - m$. Since the rep ${}_{\pi/a}E_{m,-m}$ is a self-conjugate one iff $m' = m$, that happens only for q even,

Table 11. The reps of the line groups $L(2q)_a/mcm, q = 1, 2, \dots$. For $\alpha, M(s)$ and P see table 1, for t see table 2 and for $k, K(t)$ see table 6; $r = 0, 1, \dots, q-1; m$ as in table 1 for ${}^kG_{m,-m}$ while for ${}^kG_{m,-m'}$ one has $m = 1, \dots, \frac{1}{2}(q-1)$ for q odd and $m = 1, \dots, \frac{1}{2}(q-2)$ for q even; $m' = q - m$. For $k = 0$ reps see the comment in the caption to table 9. Note that $L2_1/mcm$ has no four-dimensional reps and that for $L4_2/mcm$ ${}^{\pi/a}G_{m,-m'}$ does not appear.

Rep	$(C_{2q}^{2r} t)$	$(C_{2q}^{2r+1} \frac{1}{2}+t)$
${}^kE_{A_0}$	$K(t)$	$K(\frac{1}{2}+t)$
${}^kE_{B_0}$	$K(t)$	$K(\frac{1}{2}+t)$
${}^kG_{m,-m}$	$\begin{pmatrix} \exp(ikt\alpha)M(2r) & 0 \\ 0 & \exp(-ikt\alpha)M(2r) \end{pmatrix}$	$\begin{pmatrix} \exp[ik(\frac{1}{2}+t)\alpha]M(2r+1) & 0 \\ 0 & \exp[-ik(\frac{1}{2}+t)\alpha]M(2r+1) \end{pmatrix}$
${}^kE_{A_q}$	$K(t)$	$-K(\frac{1}{2}+t)$
${}^kE_{B_q}$	$K(t)$	$-K(\frac{1}{2}+t)$
${}^{\pi/a}E_{A_0}^A$	$(-1)^r \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$i(-1)^r \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
${}^{\pi/a}E_{B_0}^B$	$(-1)^r \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$i(-1)^r \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
${}^{\pi/a}G_{m,-m}^{m',-m'}$	$(-1)^r \begin{pmatrix} M(2r) & 0 \\ 0 & M(2r) \end{pmatrix}$	$i(-1)^r \begin{pmatrix} M(2r+1) & 0 \\ 0 & -M(2r+1) \end{pmatrix}$
${}^{\pi/a}E_{0,-0}^\pm$	$(-1)^{r+\pm} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$(-1)^{r+\pm} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

Rep	$(\sigma_0 C_{2q}^{2r} t)$	$(\sigma_0 C_{2q}^{2r+1} \frac{1}{2} + 1)$
${}^k E_{A_0}$	$K(t)$	$K(\frac{1}{2} + t)$
${}^k E_{B_0}$	$-K(t)$	$-K(\frac{1}{2} + t)$
${}^k G_{m,-m}$	$\begin{pmatrix} \exp(ikta) PM(2r) & 0 \\ 0 & \exp(-ikta) PM(2r) \end{pmatrix}$	$\begin{pmatrix} \exp[ik(\frac{1}{2} + t)a] PM(2r+1) & 0 \\ 0 & \exp[-ik(\frac{1}{2} + t)a] PM(2r+1) \end{pmatrix}$
${}^k E_{A_0}$	$K(t)$	$-K(\frac{1}{2} + t)$
${}^k E_{B_0}$	$-K(t)$	$K(\frac{1}{2} + t)$
$\pi/a E_{A_0}^{\pm}$	$(-1)^t \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$i(-1)^t \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$\pi/a E_{B_0}^{\pm}$	$-(-1)^t \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$-i(-1)^t \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$\pi/a G_{m,-m}^{\pm}$	$(-1)^t \begin{pmatrix} PM(2r) & 0 \\ 0 & PM(2r) \end{pmatrix}$	$i(-1)^t \begin{pmatrix} PM(2r+1) & 0 \\ 0 & -PM(2r+1) \end{pmatrix}$
$\pi/a E_{v,-v}^{\pm}$	$(-1)^{t+r} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$(-1)^{t+r} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Table 11—continued

Rep	$(\sigma_k C_{2q}^{2r} -t)$	$(\sigma_k C_{2q}^{2r+1} -\frac{1}{2} - t)$
${}_{-k}^k E_{A_0}$	$PK(t)$	$PK(\frac{1}{2} + t)$
${}_{-k}^k E_{B_0}$	$PK(t)$	$PK(\frac{1}{2} + t)$
${}_{-k}^k G_{m,-m}$	$\begin{pmatrix} 0 & \exp(-ikta)M(2r) \\ \exp(ikta)M(2r) & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \exp[-ik(\frac{1}{2} + t)a]M(2r+1) \\ \exp[ik(\frac{1}{2} + t)a]M(2r+1) & 0 \end{pmatrix}$
${}_{-k}^k E_{A_q}$	$PK(t)$	$-PK(\frac{1}{2} + t)$
${}_{-k}^k E_{B_q}$	$PK(t)$	$-PK(\frac{1}{2} + t)$
$\pi/a E_{A_0}^A$	$(-1)^r \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$i(-1)^r \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
$\pi/a E_{B_0}^B$	$(-1)^r \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$i(-1)^r \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
$\pi/a G_{m,-m}^{m',-m'}$	$(-1)^r \begin{pmatrix} 0 & M(2r) \\ M(2r) & 0 \end{pmatrix}$	$i(-1)^r \begin{pmatrix} 0 & -M(2r+1) \\ M(2r+1) & 0 \end{pmatrix}$
$\pi/a E_{\alpha,-\alpha}^{\pm}$	$\pm(-1)^{r+\alpha} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\pm(-1)^{r+\alpha} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Rep	$(\sigma_n \sigma_v C_{2q}^{2r} -t)$	$(\sigma_n \sigma_v C_{2q}^{2r+1} -\frac{1}{2} - t)$
$\begin{matrix} -k E_{A_0} \\ -k E_{B_0} \end{matrix}$	$\begin{matrix} PK(t) \\ -PK(t) \end{matrix}$	$\begin{matrix} PK(\frac{1}{2}+t) \\ -PK(\frac{1}{2}+t) \end{matrix}$
$-k G_{m,-m}$	$\begin{matrix} 0 \\ \exp(ikta)PM(2r) \\ 0 \end{matrix}$	$\begin{matrix} 0 \\ \exp[ik(\frac{1}{2}+t)a]PM(2r+1) \\ 0 \end{matrix}$
$\begin{matrix} -k E_{A_q} \\ -k E_{B_q} \end{matrix}$	$\begin{matrix} PK(t) \\ -PK(t) \end{matrix}$	$\begin{matrix} \exp[ik(\frac{1}{2}+t)a]PM(2r+1) \\ -PK(\frac{1}{2}+t) \\ PK(\frac{1}{2}+t) \end{matrix}$
$\pi/a E_{A_0}^A$	$(-1)^t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$i(-1)^t \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
$\pi/a E_{B_0}^B$	$-(-1)^t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$-i(-1)^t \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
$\pi/a G_{m,-m}^{m',-m'}$	$(-1)^t \begin{pmatrix} 0 & PM(2r) \\ PM(2r) & 0 \end{pmatrix}$	$i(-1)^t \begin{pmatrix} 0 & -PM(2r+1) \\ PM(2r+1) & 0 \end{pmatrix}$
$\pi/a E_{v,-v}^\dagger$	$\pm(-1)^{t+r} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\pm(-1)^{t+r} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

† For $q = 2v = 2, 4, 6, \dots$ only.

i.e. for $q = 2v$, $v = 1, 2, \dots$, $m' = m = v$. To derive the rep $\pi/a \mathbf{E}_{v,-v}$ one has to determine a matrix Z of the form (13) and satisfying (8), which here reads

$$Z(-1)^t M(2r) = (-1)^t M(2r) Z$$

$$Zi(-1)^t M(2r+1) = -i(-1)^t M(2r+1) Z$$

$$Z(-1)^t PM(2r) = (-1)^t PM(2r) Z$$

$$Zi(-1)^t PM(2r+1) = i(-1)^t PM(2r+1) Z,$$

where the latter two lines correspond to $(\sigma_v C_{2q}^{2r} | t)$ and $(\sigma_v C_{2q}^{2r+1} | \frac{1}{2} + t)$ respectively. Since for $m = v$, $n = 2q = 4v$ one has

$$M(2r) = (-1)^r \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad M(2r+1) = (-1)^r \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix},$$

one easily finds that

$$Z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = P. \quad (26)$$

(e) In all other cases $m' = q - m \neq m$ and the two reps, $\pi/a \mathbf{E}_{m,-m}$ and $\pi/a \mathbf{E}_{m',-m'}$, $m' = q - m$, induce via (14a,b) a four-dimensional rep $\pi/a \mathbf{G}_{m,-m}^{m',-m'}$ of $\mathbf{L}(2q)_q/mcm$.

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Note. The following corrections should be made to the tables of Božović *et al* (1978).

Table no	Stands	Should read
06	$-\pi/a \leq k < \pi/a$	$-\pi/a < k \leq \pi/a$
08	$(\sigma_h C_n^s t)$	$(\sigma_h C_n^s -t)$
09	$\exp(ikra/2)$ $\exp(-ikra/2)$ $k = \pi/ar$	$\exp(ika/2)$ $\exp(-ika/2)$ $k = \pi/a$
11	$(\sigma_h C_n^s f/2 + t)$ r/P	$(\sigma_h C_n^s -f/2 - t)$ P
	$(\sigma_h C_{2n} C_n^s t)$	$(\sigma_h C_{2n} C_n^s -t)$
13	$(UC_n^s t)$	$(UC_n^s -t)$
14	$(UC_n^s \text{Fr}(sp/n) + t)$	$(UC_n^s -\text{Fr}(sp/n) - t)$

References

- Blumen A and Merkel C 1977 *Phys. Stat. Solidi b* **83** 425–31
 Božović I B, Vujičić M and Herbut F 1978 *J. Phys. A: Math. Gen.* **11** 2133–47
 Delhalle J 1980 *Recent Advances in the Quantum Theory of Polymers: Lecture Notes in Physics* **113** ed. J-M André *et al* (Berlin: Springer)

- Herbut F, Vujičić M and Papadopolos Z 1980 *J. Phys. A: Math. Gen.* **13** 2577–89
- Ladik J 1978 *Excited States in Quantum Chemistry* ed. C A Nicolaides and R D Beck (Dordrecht: Reidel)
- McCubbin W L 1975 *Electronic Structure of Polymers and Molecular Crystals* ed. J-M André and J Ladik (New York: Plenum)
- Miller R L 1975 *Polymer Handbook* ed. J Bandrup and E H Immergut (New York: Wiley)
- Tobin M C 1955 *J. Chem. Phys.* **23** 891–6
- Vujičić M, Božović I B and Herbut F 1977 *J. Phys. A: Math. Gen.* **10** 1271–9