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Irreducible representations of the symmetry groups of polymer molecules I

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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 the reps of the line groups whose isogonal point groups are $\mathbf{C}_n$, $\mathbf{C}_{nv}$, $\mathbf{C}_{nh}$, $\mathbf{S}_{2n}$, and $\mathbf{D}_n$ are constructed. For some line groups the reps are obtained as products of the reps of the translational subgroup and the reps of the isogonal point group. The rest of the reps are induced from those of the corresponding invariant subgroups of index two.

1. Introduction

In a previous paper (Vujičić *et al* 1977, to be referred to as LG) we constructed the line groups, which are the symmetry groups of stereoregular polymer molecules. In fact, they describe exactly the symmetries of three-dimensional objects translationally periodic along a line. An example of such an object is a single infinite linear chain, which is the most important model in theoretical investigations of stereoregular polymer molecules.

Our method of constructing line groups proved to be very useful in the construction of all unitary irreducible representations (reps) of the line groups (Božović 1975). These reps or their characters are what is needed in many quantum mechanical treatments of physical properties of polymer molecules. We shall point out some of these applications (Božović *et al* 1976).

The symmetry properties of polymer molecules are used extensively in explaining *vibrational spectra* of these molecules (analysis by means of normal vibrations, and related processes of infrared absorption and Raman scattering). For the study of fundamental normal vibrations (wavevector $k=0$), as well as for one-phonon processes in which the change of k can be neglected, one can make use of an approximate symmetry—the factor group $\mathbf{L}/\mathbf{T}$, where $\mathbf{L}$ is the line group and $\mathbf{T}$ its translational subgroup. This means that one can utilise reps of the isogonal point group $\mathbf{P}$ isomorphic to $\mathbf{L}/\mathbf{T}$ instead of reps of line groups $\mathbf{L}$. One can find examples of using the factor group symmetries in Tobin (1955), Krimm (1960), Zbinden (1964), Elliott (1969), and Oleinik and Kompaneyets (1968).

However, when the wavevector k is different from zero (non-fundamental normal vibrations, two-phonon and multiphonon processes) one needs reps of line groups

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(Higgs 1953, Tobin 1960). Data about such processes have become available due to neutron diffraction experiments (Allen 1972). The selection rules for two-phonon processes are important and should be investigated.

Reps of crystallographic space groups have been used extensively in the analysis of the *electron band structure* of crystals (Slater 1972, Jannsen 1973, Lax 1974). The reps of the line groups can be expected to be even more useful in investigating electron spectra of polymer molecules (for infinite polymer chains, unlike in the case of crystals, the k vectors possessing symmetry usually outnumber the rest). There has been a great number of papers dealing with electron energy spectra (band structure) for polymer molecules in recent years. This progress has been made possible by the development of very elaborate computer programs for different semi-empirical and *ab initio* (Hartree–Fock) calculations developed by Ladik and co-workers, and André and co-workers (André and Ladik 1975) etc. In these calculations symmetries (apart from the translational ones) have been made very little use of (some of the line groups were employed by McCubbin 1975 and Merkel 1977). The reps of the line groups can provide us with symmetry-adapted basis functions for self-consistent calculations, make them much faster and easier, and furnish us with a symmetry labelling for energy bands, as well as give selection rules for different processes, etc. However, up to now reps of line groups have been published, to our knowledge, only for the simplest of the line groups (Tobin 1960, McCubbin 1975, Merkel 1977). It is the aim of the present work to fill that gap to some extent (deriving all the reps of the line groups whose isogonal point groups are $\mathbf{C}_n$, $\mathbf{C}_{nv}$, $\mathbf{C}_{nh}$, $\mathbf{S}_{2n}$, and $\mathbf{D}_n$) and to make possible more extensive use of symmetries in polymer physics. In the next paper in this series we shall complete this task by giving the reps for the line groups whose isogonal point groups are $\mathbf{D}_{nd}$ and $\mathbf{D}_{nh}$.

In the case when the Hamiltonian is invariant under time reversal θ, the symmetry group is enlarged: $\mathbf{L}+\theta\mathbf{L}$. It is interesting to learn if the degeneracy of the levels is doubled or not. In a forthcoming paper we shall apply Herring's criterion (Herring 1937) to all reps of line groups to find the answer to the problem of the degeneracy of levels.

2. Method of construction of reps

Every line group $\mathbf{L}$ has an invariant subgroup $\mathbf{T}$ consisting of one-dimensional pure translations (cf LG):

$$\mathbf{T}=\{(E|t)|t=0, \pm1, \pm2, \ldots\}, \tag{1}$$

where E is the unit element in the isogonal point group $\mathbf{P}\cong\mathbf{L}/\mathbf{T}$. $\mathbf{T}$ is cyclic and its reps are easily found:

$$d_k(E|t)=\exp(\mathrm{i}kta), \tag{2}$$

where a is the translational period, and k takes on the values from the interval $(-\pi/a, \pi/a]$—the first Brillouin zone†.

† The translational group is usually made finite by means of the periodic (or Born–von Kármán) boundary conditions: $(E|N)=(E|0)$, where N is an arbitrary large integer (Streitwolf 1971). Then k takes on only N values from $(-\pi/a, \pi/a]$. Hence finite-group theory can be used.

Each line group $\mathbf{L}$ can be expressed as the sum of $|\mathbf{P}|$ cosets of $\mathbf{T}$:

$$\mathbf{L}=\sum_i (R_i|v_i)\mathbf{T}, \tag{3}$$

where $v_i \in [0, 1)$ are fractional translations, and $R_i \in \mathbf{P}$ (cf LG). Every point group $\mathbf{P}$ isogonal to a line group is axial, i.e. it leaves the line of translations invariant. Its elements R can be of two types: of R^+ type if $R\boldsymbol{a}=\boldsymbol{a}$, or of R^- type if $R\boldsymbol{a}=-\boldsymbol{a}$. A line group in which all R_i in (3) are of R^+ type is called of $\mathbf{L}^+$ type itself. Otherwise, half of the R_i are R^+ and the other half R^-, and then the line group is called of $\mathbf{L}^-$ type. The reps of line groups are found in this paper differently for groups of $\mathbf{L}^+$ type and differently for those of $\mathbf{L}^-$ type.

2.1. *Reps of line groups of* $\boldsymbol{L}^+$ *type*

To begin with, one may try to construct reps of a line group of $\mathbf{L}^+$ type by multiplying reps $\boldsymbol{d}_k(\mathbf{T})$ (cf (2)) of the translational subgroup $\mathbf{T}$ and reps $\boldsymbol{D}_m(\mathbf{P})$ of the isogonal point group $\mathbf{P}$, with an extra factor $\exp(ikva)$ when the group is non-symmorphic:

$${}_kD_m(R|v+t)=\exp[ik(v+t)a]D_m(R). \tag{4}$$

The requirement of homomorphism gives

$${}_kD_m(R|v+t)\,{}_kD_m(Q|w+s)={}_kD_m(RQ|v+t+Rw+Rs).$$

This is obviously fulfilled if

$$\exp[ik(w+s)a]=\exp[ik(Rw+Rs)a], \tag{5}$$

and this is indeed satisfied since all rotations R in $\mathbf{L}^+$ are of R^+ type. The irreducibility of ${}_k\boldsymbol{D}_m(\mathbf{L}^+)$ follows from that of $\boldsymbol{D}_m(\mathbf{P})$, as the $\boldsymbol{d}_k(\mathbf{T})$ are one-dimensional. Two reps ${}_k\boldsymbol{D}_m(\mathbf{L}^+)$ and ${}_{k'}\boldsymbol{D}_{m'}(\mathbf{L}^+)$ are equivalent, i.e. their characters are equal, if and only if $k=k'$ and $m=m'$. If one has a complete set of reps $\boldsymbol{D}_m(\mathbf{P})$, then construction (4) gives a complete set of reps for $\mathbf{L}^+$. This is easily proved if one applies the Burnside theorem:

$$\sum_k\sum_m (\dim {}_k\boldsymbol{D}_m(\mathbf{L}^+))^2=N\sum_m (\dim \boldsymbol{D}_m(\mathbf{P}))^2=N|\mathbf{P}|=|\mathbf{L}^+|.$$

Therefore, in order to obtain a complete set of non-equivalent reps of any line group of $\mathbf{L}^+$ type, it is sufficient to know all the reps of the corresponding isogonal axial point group ($\mathbf{C}_n$ or $\mathbf{C}_{nv}$, $n=1,2,\ldots$, cf LG). Though they are known in the literature, we derive them in this work by the same method as for line groups and achieve a concise form, unique for each family of point groups (i.e. for those differing in the order of the main axis only). This form shortens immensely our derivation of the reps of the line groups.

2.2. *Reps of line groups of* $\boldsymbol{L}^-$ *type*

Each line group of $\mathbf{L}^-$ type can be written as (cf LG):

$$\mathbf{L}^-=\mathbf{L}^++(R^-|0)\mathbf{L}^+. \tag{6}$$

Reps of $\mathbf{L}^-$ can be induced from those of its invariant subgroup $\mathbf{L}^+$. For this besides

${}_k\boldsymbol{D}_m(\mathbf{L}^+)$ we need its conjugate rep ${}_k\bar{\boldsymbol{D}}_m(\mathbf{L}^+)$ defined by

$$ {}_k\bar{D}_m(R^+|v+t) \equiv {}_kD_m[(R^-|0)(R^+|v+t)(R^-|0)^{-1}]. \tag{7}$$

If the two reps ${}_k\boldsymbol{D}_m(\mathbf{L}^+)$ and ${}_k\bar{\boldsymbol{D}}_m(\mathbf{L}^+) = {}_{\bar{k}}\boldsymbol{D}_{\bar{m}}(\mathbf{L}^+)$ are not equivalent, then from the two of them one can induce one rep of $\mathbf{L}^-$ and we denote it by ${}^{\bar{k}}_{k}\boldsymbol{Q}^{\bar{m}}_{m}(\mathbf{L}^-)$ (the induction procedure is explained in Jansen and Boon 1967):

$$ {}^{\bar{k}}_{k}Q^{\bar{m}}_{m}(R^+|v+t) = \begin{pmatrix} {}_kD_m(R^+|v+t) & 0 \\ 0 & {}_{\bar{k}}D_{\bar{m}}(R^+|v+t) \end{pmatrix}, \tag{8a}$$

$$ {}^{\bar{k}}_{k}Q^{\bar{m}}_{m}(R^-R^+|-v-t) = \begin{pmatrix} 0 & {}_{\bar{k}}D_{\bar{m}}(R^+|v+t) \\ {}_kD_m((R^-)^2R^+|v+t) & 0 \end{pmatrix}. \tag{8b}$$

Obviously,

$$ (R^-R^+|-v-t) = (R^-|0)(R^+|v+t), $$

and

$$ {}^{\bar{k}}_{k}Q^{\bar{m}}_{m}(R^-R^+|v-t) = P\,{}^{k}_{k}Q^{m}_{m}(R^+|v+t), $$

where

$$ P \equiv \begin{pmatrix} 0 & I \\ D_m(R^-)^2 & 0 \end{pmatrix} $$

and I is the unit matrix of the same dimension as ${}_kD_m$, P being the representative of $(R^-|0)$. The other possible rep ${}^{k}_{\bar{k}}\boldsymbol{Q}^{m}_{\bar{m}}(\mathbf{L}^-)$ obtainable in this way from the same two reps ${}_{\bar{k}}\boldsymbol{D}_{\bar{m}}(\mathbf{L}^+)$ and ${}_k\boldsymbol{D}_m(\mathbf{L}^+)$ is obviously equivalent to ${}^{\bar{k}}_{k}\boldsymbol{Q}^{\bar{m}}_{m}$they have the same characters. In the actual construction of the reps below we evaluate $\bar{k}$ and $\bar{m}$ as functions of k and m respectively, and restrict the latter to suitable intervals so that each ${}^{\bar{k}}_{k}\boldsymbol{Q}^{\bar{m}}_{m}$ appears only once.

If we take two different pairs of conjugate and non-equivalent reps of $\mathbf{L}^+$, then the reps of $\mathbf{L}^-$ which are furnished by them are not equivalent (Zak 1960).

The mutally conjugate reps ${}_k\boldsymbol{D}_m(\mathbf{L}^+)$ and ${}_{\bar{k}}\boldsymbol{D}_{\bar{m}}(\mathbf{L}^+)$ are not equivalent when $k \neq 0$ and $k \neq \pi/a$. Proof is easily obtained since for all $(R^+|v+t) \in \mathbf{L}^+$ the requirement

$$ {}_k\boldsymbol{D}_m(\mathbf{L}^+) \sim {}_k\bar{\boldsymbol{D}}_m(\mathbf{L}^+) $$

implies equality of characters, which in turn gives

$$ \chi_m(R^-R^+(R^-)^{-1})/\chi_m(R^+) = \exp[2ik(v+t)a], \tag{9}$$

where χ_m is the character of the rep $\boldsymbol{D}_m$ of the isogonal point group of $\mathbf{L}^+$. But this is not true (because only one side depends on t) unless $k=0$ or $k=\pi/a$ (with $v=0$). Therefore, the reps of $\mathbf{L}^-$ for $k \neq 0$ and $k \neq \pi/a$ can always be obtained by induction from those of $\mathbf{L}^+$ by means of the construction (8a, b).

For $k=0$ condition (5) is fulfilled so that for this point the reps of $\mathbf{L}^-$ are the same as the reps of its isogonal point group (see (4)):

$$ {}_0D_m(R|v+t) = D_m(R), \tag{10}$$

for all $(R|v+t) \in \mathbf{L}^-$.

For $k=\pi/a$, let us consider first the symmorphic line groups, i.e. those which are semi-direct products of their translational and rotational subgroups $\mathbf{L} = \mathbf{T} \wedge \mathbf{P}$. In this case condition (5) is satisfied since the fractional translations are all zero. Hence, construction (4) can be applied in this case too:

$$ {}_{\pi/a}D_m(R|t) = (-1)^t D_m(R) \qquad (11) $$

for all $(R|t) \in \mathbf{L}$.

For non-symmorphic line groups, on the other hand, condition (5) is not satisfied and one has to check for each of them and for every m whether ${}_{\pi/a}\boldsymbol{D}_m(\mathbf{L}^+)$ and ${}_{\pi/a}\bar{\boldsymbol{D}}_m(\mathbf{L}^+)$ are equivalent or not. If they are not equivalent one applies construction (8a, b). If they are equivalent, i.e. if ${}_{\pi/a}\boldsymbol{D}_m(\mathbf{L}^+)$ is self-conjugate, then we take resort to the fact that $(R^-|0)$ in (6) is of order two in all these groups, so that the line group $\mathbf{L}^-$ is a semi-direct product of its two subgroups: $\mathbf{L}^+$ and the cyclic one $\mathbf{J} \equiv \{(E|0), (R^-|0)\}$. Then the two reps ${}_k\boldsymbol{D}^{\pm}_m(\mathbf{L}^-)$ can be constructed in a direct-product-like manner (Jansen and Boon 1967):

$$ {}_kD^{\pm}_m(R^+|v+t) = {}_kD_m(R^+|v+t), \qquad (12a) $$

$$ {}_kD^{\pm}_m(R^-R^+|-v-t) = \pm {}_kD_m(R^+|v+t). \qquad (12b) $$

This construction reflects the fact that the cyclic subgroup $\mathbf{J}$ has only two one-dimensional reps, $\{1, 1\}$ and $\{1, -1\}$. Therefore, every self-conjugate rep of $\mathbf{L}^+$ gives two non-equivalent reps of $\mathbf{L}^-$ (Zak 1960).

In the manner described above one obtains a complete set of non-equivalent reps of $\mathbf{L}^-$, and this can be proved by using the Burnside theorem:

$$ \sum_m (\dim {}_0\boldsymbol{D}_m(\mathbf{L}^-))^2 + \sum_{0<k<\pi/a} \sum_m (\dim {}^{\bar{k}}_k\boldsymbol{Q}^{\bar{m}}_m(\mathbf{L}^-))^2 + \sum_{m'} (\dim {}_{\pi/a}\boldsymbol{D}^{\pm}_{m'}(\mathbf{L}^-))^2 $$
$$ + \sum_{m''} (\dim {}_{\pi/a}\boldsymbol{Q}^{\bar{m}''}_{m''}(\mathbf{L}^-))^2 $$
$$ = |\mathbf{P}^-| + (N/2-1)4|\mathbf{P}^+| + 2|\mathbf{P}^+| = N|\mathbf{P}^-| = |\mathbf{L}^-|, $$

where m' and m'' enumerate for $k = \pi/a$ the self-conjugate reps and those which are not, respectively; and $\mathbf{P}^-$ and $\mathbf{P}^+$ are the isogonal point groups of $\mathbf{L}^-$ and $\mathbf{L}^+$, respectively, and therefore $|\mathbf{P}^-| = 2|\mathbf{P}^+|$.

3. Construction of the reps of the line groups of $\mathbf{L}^+$ type

3.1. Reps of the line groups whose isogonal point groups are $\boldsymbol{C}_n$, $n = 1, 2, 3, \ldots$

The point groups $\mathbf{C}_n$ are cyclic, so that the general form of their elements is C^s_n, $s = 0, 1, \ldots, n-1$, where C_n is a rotation through $\alpha = 2\pi/n$ around the z axis. The complete set of reps for $\mathbf{C}_n$ is obviously given by

$$ A_m(C^s_n) = \exp(\mathrm{i}ms\alpha), \qquad (13) $$

where $\mathbf{A}$ always denotes one-dimensional reps, and m takes on n values†:

$$ m = \begin{cases} 0, \pm 1, \pm 2, \ldots, \pm(n-1)/2 & \text{if } n \text{ is odd} \qquad (14) \\ 0, \pm 1, \pm 2, \ldots, \pm(n-2)/2, n/2 & \text{if } n \text{ is even.} \qquad (15) \end{cases} $$

Note that the rep with $m = -n/2$ (for n even) is the same as that with $m = n/2$.

† This choice of the range of m is such that the action of the operators σ_v, U, and θ is as simple as possible. Hence, the mutally conjugate indices m and $\bar{m}$ are easily found, and, in most cases, differ in sign only (cf (17), (24), and (25)).

There are two families† of line groups whose isogonal point groups are $\mathbf{C}_n$: $\mathbf{L}n$, $n = 1, 2, 3, \ldots$ (note that $\mathbf{L}1 = \mathbf{T}$), and $\mathbf{L}n_p$, $n = 2, 3, 4, \ldots$, $p = 1, 2, \ldots, n-1$ (cf LG). The corresponding general forms of the elements are: $(C_n^s|t)$ and $(C_n^s|\mathrm{Fr}(sp/n)+t)$, where $\mathrm{Fr}(x)$ denotes the fractional part of x (cf LG). A special case is $\mathbf{L}(2q)_q$, where $n = 2q$, $q = 1, 2, 3, \ldots$ and $p = q$, when the general form of the elements is $(C_n^s|f/2+t)$, where $f = 0$ if s is even and $f = 1$ if s is odd (cf below the line groups $\mathbf{L}(2q)_q mc$ and $\mathbf{L}(2q)_q/m$, that have $\mathbf{L}(2q)_q$ as their invariant subgroup).

For the construction of the reps we use formula (4) with (13):

$$ {}_kA_m(C_n^s|\mathrm{Fr}(sp/n)+t) = \exp\{\mathrm{i}k[\mathrm{Fr}(sp/n)+t]a\}\exp(\mathrm{i}ms\alpha). \qquad (16) $$

For $p = 0$ (16) gives the reps of $\mathbf{L}n$, and for $p = 1, 2, \ldots, n-1$ those of $\mathbf{L}n_p$. For $k = 0$ and $k = \pi/a$ one has somewhat simpler forms exhibited in tables 1 and 2.

Table 1. The reps of the line groups $\mathbf{L}n$, $n = 1, 2, 3, \ldots$ (cf (16)) with $\alpha = 2\pi/n$, $s = 0, 1, \ldots, n-1$; for m see (14) and (15).

k	reps	$(C_n^s\vert t)$
0	${}_0A_m$	$\exp(\mathrm{i}ms\alpha)$
$0<\vert k\vert<\pi/a$	${}_kA_m$	$\exp(\mathrm{i}kta)\exp(\mathrm{i}ms\alpha)$
π/a	${}_{\pi/a}A_m$	$(-1)^t\exp(\mathrm{i}ms\alpha)$

Table 2. The reps of the line groups $\mathbf{L}n_p$, $n = 2, 3, 4, \ldots$, $p = 1, 2, \ldots, n-1$ (cf (16)), for α, s and m see the caption of table 1. In the special cases when $n = 2q$, $p = q$, $q = 1, 2, 3, \ldots$, $\mathrm{Fr}(sp/n) = f/2$, where $f = 0$ for s even, and $f = 1$ for s odd.

k	reps	$(C_n^s\vert\mathrm{Fr}(sp/n)+t)$
0	${}_0A_m$	$\exp(\mathrm{i}ms\alpha)$
$0<\vert k\vert<\pi/a$	${}_kA_m$	$\exp\{\mathrm{i}k(\mathrm{Fr}(sp/n)+t]a\}\exp(\mathrm{i}ms\alpha)$
π/a	${}_{\pi/a}A_m$	$(-1)^{\mathrm{Fr}(sp/n)+t}\exp(\mathrm{i}ms\alpha)$

3.2. *Reps of the line groups whose isogonal point groups are $\mathbf{C}_{nv}$, $n = 1, 2, 3, \ldots$*

The point groups $\mathbf{C}_{nv}$, $n = 2, 3, 4, \ldots$ are obtained as semi-direct products of the corresponding point group $\mathbf{C}_n$ with $\mathbf{C}_{1v} = \{E, \sigma_v\}$, where σ_v is the reflection in a vertical plane (containing the z axis):

$$ \mathbf{C}_{nv} = \mathbf{C}_n \wedge \mathbf{C}_{1v} = \mathbf{C}_n + \sigma_v\mathbf{C}_n, \qquad n = 2, 3, 4, \ldots $$

(cf LG). Consequently, the general form of the elements is either C_n^s or $\sigma_v C_n^s$, $n = 1, 2, 3, \ldots$, $s = 0, 1, \ldots, n-1$. The reps of $\mathbf{C}_{nv}$ are obtained from those of $\mathbf{C}_n$ by induction (in analogy with (8a, b)) or in a direct-product-like manner (in analogy with (12a, b)). For that we have to conjugate each rep $\mathbf{A}_m(\mathbf{C}_n)$ (equation (13)) by σ_v and

† We call a family that set of line groups (differing in the value of n and possibly in the symbols by which they are denoted) for which the general form of elements is the same, i.e. each row in table 1 of LG.

find out which are the conjugate pairs and which are the self-conjugate reps. We thus obtain

$$\bar{A}_m(C_n^s) = A_m(\sigma_v C_n^s \sigma_v^{-1}) = A_m(C_n^{-s}) = A_{-m}(C_n^s), \tag{17}$$

which is a consequence of the generator relation $C_n\sigma_v = \sigma_v C_n^{n-1}$ for $\mathbf{C}_{nv}$. From (13) and (17) it follows that:

(i) $\mathbf{A}_0(\mathbf{C}_n) = \bar{\mathbf{A}}_0(\mathbf{C}_n)$—a self-conjugate rep;

(ii) $\mathbf{A}_m(\mathbf{C}_n)$ and $\mathbf{A}_{-m}(\mathbf{C}_n) = \bar{\mathbf{A}}_m(\mathbf{C}_n)$—a pair of conjugate reps

$$\text{for} \quad m = 1, 2, \ldots, (n-1)/2 \quad \text{if} \quad n = 3, 5, 7, \ldots \tag{18a}$$

$$\text{or} \quad m = 1, 2, \ldots, (n-2)/2 \quad \text{if} \quad n = 4, 6, 8, \ldots; \tag{18b}$$

(iii) $\mathbf{A}_{n/2}(\mathbf{C}_n) = \bar{\mathbf{A}}_{n/2}(\mathbf{C}_n)$—a self-conjugate rep for n even (see the remark after (15)).

Each self-conjugate one-dimensional rep of $\mathbf{C}_n$ furnishes two one-dimensional reps for $\mathbf{C}_{nv}$ (cf (12*a*, *b*)), which we shall denote by **A** (when σ_v is represented by 1) and by **B** (when σ_v is represented by -1). Each pair of conjugate reps $\mathbf{A}_m$, $\mathbf{A}_{-m}$ of $\mathbf{C}_n$ will give one two-dimensional rep $\mathbf{E}_{m,-m}$ (cf (8*a*, *b*)) of $\mathbf{C}_{nv}$ (see table 3). Note that for $\mathbf{C}_{1v}$ and $\mathbf{C}_{2v}$ there are no two-dimensional reps (cf (18*a*, *b*)).

Table 3. The reps of the point groups $\mathbf{C}_{nv}$, $n = 1, 2, 3, \ldots$, where $\alpha = 2\pi/n$, $s = 0, 1, \ldots, n-1$, and the range of m is specified by (18*a*, *b*),

$$M = \begin{pmatrix} \exp(\mathrm{i}ms\alpha) & 0 \\ 0 & \exp(-\mathrm{i}ms\alpha) \end{pmatrix}, \qquad P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

reps	C_n^s	$\sigma_v C_n^s$
A_0	1	1
B_0	1	-1
$E_{m,-m}$	M	PM
	and only for $n = 2, 4, 6, \ldots$	
$A_{n/2}$	$(-1)^s$	$(-1)^s$
$B_{n/2}$	$(-1)^s$	$-(-1)^s$

There are three families of line groups whose isogonal point groups are $\mathbf{C}_{nv}$ (cf LG):

	n odd	n even	general form of the elements
(1)	**L***nm*	**L***nmm*	$(C_n^s\|t)$, $(\sigma_v C_n^s\|t)$
(2)	**L***nc*	**L***ncc*	$(C_n^s\|t)$, $(\sigma_v C_n^s\|1/2+t)$
(3)		$\mathbf{L}(2q)_q mc$	$(C_n^s\|f/2+t)$, $(\sigma_v C_n^s\|f/2+t)$†

† In contrast to table 1 of LG here we use f (see the caption of table 2) because it makes the presentation of the reps considerably more compact (see tables 6 and 9). It should be noted that in table 1 of LG the integer $2r$ was always misprinted as 2_r.

The reps of these line groups are obtained (tables 4, 5 and 6) by construction (4).

Table 4. The reps of the line groups **L**nm, $n = 1, 3, 5, \ldots$ and **L**nmm, $n = 2, 4, 6, \ldots$. For α, s, m, M, and P see the caption of table 3.

k	reps	$(C_n^s\|t)$	$(\sigma_v C_n^s\|t)$
$-\pi/a < k \leq \pi/a$	${}_kA_0$	$\exp(ikta)$	$\exp(ikta)$
$-\pi/a < k \leq \pi/a$	${}_kB_0$	$\exp(ikta)$	$-\exp(ikta)$
$-\pi/a < k \leq \pi/a$	${}_kE_{m,-m}$	$\exp(ikta)M$	$\exp(ikta)PM$
	and only for $n = 2, 4, 6, \ldots$		
$-\pi/a < k \leq \pi/a$	${}_kA_{n/2}$	$(-1)^s \exp(ikta)$	$(-1)^s \exp(ikta)$
$-\pi/a < k \leq \pi/a$	${}_kB_{n/2}$	$(-1)^s \exp(ikta)$	$-(-1)^s \exp(ikta)$

Note that in the case of **L**$1m$ and **L**$2mm$ there are no two-dimensional reps (cf the note below table 3).

Table 5. The reps of the line groups **L**nc, $n = 1, 3, 5, \ldots$ and **L**ncc, $n = 2, 4, 6, \ldots$. Concerning α, s, m, M, and P see the caption of table 3.

k	reps	$(C_n^s\|t)$	$(\sigma_v C_n^s\|1/2+t)$
$-\pi/a < k \leq \pi/a$	${}_kA_0$	$\exp(ikta)$	$\exp[ik(1/2+t)a]$
$-\pi/a < k \leq \pi/a$	${}_kB_0$	$\exp(ikta)$	$-\exp[ik(1/2+t)a]$
$-\pi/a < k \leq \pi/a$	${}_kE_{m,-m}$	$\exp(ikta)M$	$\exp[ik(1/2+t)a]PM$
	and only for $n = 2, 4, 6, \ldots$		
$-\pi/a < k \leq \pi/a$	${}_kA_{n/2}$	$(-1)^s \exp(ikta)$	$(-1)^s \exp[ik(1/2+t)a]$
$-\pi/a < k \leq \pi/a$	${}_kB_{n/2}$	$(-1)^s \exp(ikta)$	$-(-1)^s \exp[ik(1/2+t)a]$

For $k = \pi/a$, $\exp(ikta) = (-1)^t$, $\exp[ik(1/2+t)a] = i(-1)^t$. Note that in the case of **L**$1c$ and **L**$2cc$ there are no two-dimensional reps.

Table 6. The reps of the line groups **L**$(2q)_q mc$, $n = 2q = 2, 4, 6, \ldots$ As to α, s, m, M, and P see the caption of table 3. Concerning f see the caption of table 2.

k	reps	$(C_n^s\|f/2+t)$	$(\sigma_v C_n^s\|f/2+t)$
$-\pi/a \leq k \leq \pi/a$	${}_kA_0$	$\exp[ik(f/2+t)a]$	$\exp[ik(f/2+t)a]$
	${}_kB_0$	$\exp[ik(f/2+t)a]$	$-\exp[ik(f/2+t)a]$
	${}_kE_{m,-m}$	$\exp[ik(f/2+t)a]M$	$\exp[ik(f/2+t)a]PM$
	${}_kA_{n/2}$	$(-1)^s \exp[ik(f/2+t)a]$	$(-1)^s \exp[ik(f/2+t)a]$
	${}_kB_{n/2}$	$(-1)^s \exp[ik(f/2+t)a]$	$-(-1)^s \exp[ik(f/2+t)a]$

For $k = \pi/ar$, $\exp[ik(f/2+t)a] = i^f(-1)^t$. Note that in the case of **L**2_1mc there are no two-dimensional reps.

4. Construction of the reps of the line groups of $\mathbf{L}^-$ type

4.1. Reps of the line groups whose isogonal point groups are $\mathbf{C}_{nh}$, $n = 1, 2, 3, \ldots$

The point groups $\mathbf{C}_{nh}$, $n = 2, 3, 4, \ldots$ can be obtained as direct products of the corresponding point groups $\mathbf{C}_n$ with $\mathbf{C}_{1h} = \{E, \sigma_h\}$, where σ_h is the reflection in the horizontal, i.e. xy plane:

$$\mathbf{C}_{nh} = \mathbf{C}_n \otimes \mathbf{C}_{1h} = \mathbf{C}_n + \sigma_h \mathbf{C}_n, \qquad n = 2, 3, 4, \ldots$$

(cf LG). Therefore, the general form of the elements of $\mathbf{C}_{nh}$ is either C_n^s or $\sigma_h C_n^s$, $n = 1, 2, 3, \ldots, s = 0, 1, \ldots, n-1$. All the reps of $\mathbf{C}_n$ are self-conjugate with respect to $\mathbf{C}_{nh}$, because σ_h commutes with the rotations C_n^s. Hence, the reps of $\mathbf{C}_{nh}$ are constructed by a method analogous to $(12a, b)$ Note that all the reps are one-dimensional since the groups are Abelian.

Table 7. The reps of the point groups $\mathbf{C}_{nh}$, $n = 1, 2, 3, \ldots$. For α, s, and m see the caption of table 1.

reps	C_n^s	$\sigma_h C_n^s$
$A_m^{\pm}$	$\exp(\mathrm{i}ms\alpha)$	$\pm\exp(\mathrm{i}ms\alpha)$

There are two families of line groups whose isogonal point groups are $\mathbf{C}_{nh}$ (see LG):

(1) $\mathbf{L}n/m = \mathbf{L}n + (\sigma_h|0)\mathbf{L}n$, $n = 1, 2, 3, \ldots$ with the general form of the elements $(C_n^s|t)$ and $(\sigma_h C_n^s|t)$;

(2) $\mathbf{L}(2q)_q/m = \mathbf{L}(2q)_q + (\sigma_h|0)\mathbf{L}(2q)_q$, $n = 2q = 2, 4, 6, \ldots$ with the general form of the elements $(C_n^s|f/2+t)$, $(\sigma_h C_n^s|f/2+t)$.

For $k = 0$ the reps ${}_0\boldsymbol{A}_m^{\pm}$ of the above line groups are the same as $\boldsymbol{A}_m^{\pm}$ of the corresponding point groups $\mathbf{C}_{nh}$ (see table 7).

For $0 < |k| < \pi/a$ one has the conjugate reps (see table 1):

$$ {}_k\bar{A}_m(C_n^s|t) = \exp(-\mathrm{i}kta)\exp(\mathrm{i}ms\alpha) = {}_{-k}A_m(C_n^s|t), \tag{19}$$

since $(\sigma_h|0)(C_n^s|t)(\sigma_h|0)^{-1} = (C_n^s|-t)$. Similarly (see table 2),

$$ {}_k\bar{A}_m(C_n^s|f/2+t) = \exp(-\mathrm{i}kta)\exp(-\mathrm{i}fka/2)\exp(\mathrm{i}ms\alpha) = {}_{-k}A_m(C_n^s|f/2+t), \tag{20}$$

since $(\sigma_h|0)(C_n^s|f/2+t)(\sigma_h|0)^{-1} = (C_n^s|-f/2+t)$.

The two reps ${}_k\boldsymbol{A}_m$ and ${}_{-k}\boldsymbol{A}_m$ of $\mathbf{L}n$ and $\mathbf{L}(2q)_q$ give rise to a two-dimensional rep (via $(8a, b)$) of $\mathbf{L}n/m$ and $\mathbf{L}(2q)_q/m$, respectively, which we denote by ${}^{-k}_{k}\boldsymbol{E}_m$. We limit k to the interval $(0, \pi/a)$, so that $-k$ belongs to $(-\pi/a, 0)$.

For $k = \pi/a$ we have to analyse separately the case of $\mathbf{L}n/m$ and separately that of $\mathbf{L}(2q)_q/m$. The line groups $\mathbf{L}n/m$ are symmorphic (table 8), hence their reps for $k = \pi/a$ are constructed according to (11). As to $\mathbf{L}(2q)_q/m$ (table 9), we have to conjugate ${}_{\pi/a}A_m(C_n^s|f/2+t) = \mathrm{i}^f(-1)^t\exp(\mathrm{i}ms\alpha)$ (cf table 2) by $(\sigma_h|0)$. One gets

$$ {}_{\pi/a}\bar{A}_m(C_n^s|f/2+t) = (-\mathrm{i})^f(-1)^t\exp(\mathrm{i}ms\alpha) = \mathrm{i}^f(-1)^t\exp[\mathrm{i}(m-q)s\alpha], \tag{21}$$

since $(-\mathrm{i})^f = \mathrm{i}^f(-1)^s = \mathrm{i}^f\exp(-\mathrm{i}qs\alpha)$.

Therefore, ${}_{\pi/a}\boldsymbol{A}_m(\mathbf{L}(2q)_q)$ and ${}_{\pi/a}\boldsymbol{A}_{m-q}(\mathbf{L}(2q)_q)$ are two conjugate reps for which m runs through the values $1, 2, \ldots, q$ (i.e. $m > 0$, cf (15)), and $m-q$ takes on the other half of values in (15).

Table 8. The reps of the line groups $\mathbf{L}n/m$, $n = 1, 2, 3, \ldots$ (see (10), table 7, (8*a*, *b*), (19) and (11)). For α, s, and m see caption of table 1;

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad K = \begin{pmatrix} \exp(\mathrm{i}kta) & 0 \\ 0 & \exp(-\mathrm{i}kta) \end{pmatrix}.$$

k	reps	$(C_n^s \mid t)$	$(\sigma_h C_n^s \mid t)$
0	${}_0A_m^{\pm}$	$\exp(\mathrm{i}ms\alpha)$	$\pm\exp(\mathrm{i}ms\alpha)$
$0<k<\pi/a$	${}_k^{-k}E_m$	$\exp(\mathrm{i}ms\alpha)K$	$\exp(\mathrm{i}ms\alpha)PK$
π/a	${}_{\pi/a}A_m^{\pm}$	$(-1)^t\exp(\mathrm{i}ms\alpha)$	$\pm(-1)^t\exp(\mathrm{i}ms\alpha)$

Table 9. The reps of the line groups $\mathbf{L}(2q)_q/m$, $n = 2q = 2, 4, 6, \ldots$ (see (10), table 7, (8*a*, *b*), (20) and (21)). For α and s see the caption of table 1, for P and K that of table 8, for f that of table 2,

$$Q = \begin{pmatrix} \exp(\mathrm{i}kra/2) & 0 \\ 0 & \exp(-\mathrm{i}kra/2) \end{pmatrix}, \qquad S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The range of m is given by (15), except for $k = \pi/ar$, where m runs through only the positive half of the interval.

k	reps	$(C_n^s \mid f/2+t)$	$(\sigma_h C_n^s \mid f/2+t)$
0	${}_0A_m^{\pm}$	$\exp(\mathrm{i}ms\alpha)$	$\pm\exp(\mathrm{i}ms\alpha)$
$0<k<\pi/a$	${}_k^{-k}E_m$	$\exp(\mathrm{i}ms\alpha)KQ^f$	$\exp(\mathrm{i}ms\alpha)PKQ^f$
π/a	${}_{\pi/a}E_m^{m-q}$	$\exp(\mathrm{i}ms\alpha)(-1)^t(\mathrm{i}S)^f$	$\exp(\mathrm{i}ms\alpha)(-1)^tP(\mathrm{i}S)^f$

4.2. *Reps of the line groups whose isogonal point groups are $\mathbf{S}_{2n}$, $n = 1, 2, 3, \ldots$*

A point group $\mathbf{S}_{2n}$ is a cyclic group of order $2n$ generated by $\sigma_h C_{2n}$. Since $(\sigma_h C_{2n})^{2s} = C_{2n}^{2s} = C_n^s$ and $(\sigma_h C_{2n})^{2s+1} = \sigma_h C_{2n}^{2s+1} = \sigma_h C_{2n} C_n^s$ $(s = 0, 1, \ldots, n-1)$, the group $\mathbf{S}_{2n}$ has an invariant subgroup $\mathbf{C}_n$, so that

$$\mathbf{S}_{2n} = \mathbf{C}_n + (\sigma_h C_{2n})\mathbf{C}_n$$

(see LG). The generator $\sigma_h C_{2n}$ can be represented by each of the $2n$ roots of one:

$$A_j(\sigma_h C_{2n}) = \exp(\mathrm{i}j2\pi/2n), \qquad j = 1, 2, \ldots, 2n.$$

For convenience we separate them into two sets and label them differently in order to preserve form (13) of the reps of the subgroup $\mathbf{C}_n$ unaltered: $A_m^+(\sigma_h C_{2n}) = \exp(\mathrm{i}m\alpha/2)$, where m takes on n values (see (14) and (15)); $A_m^-(\sigma_h C_{2n}) = \exp[\mathrm{i}(m+n)\alpha/2] = -\exp(\mathrm{i}m\alpha/2)$, which represent the remaining n roots distinct from A_m^+. The other elements of $\mathbf{S}_{2n}$ are represented by: $[\exp(\mathrm{i}m\alpha/2)]^{2s} = \exp(\mathrm{i}ms\alpha)$ and $[\exp(\mathrm{i}m\alpha/2)]^{2s+1} = \exp[\mathrm{i}m(s+1/2)\alpha]$ in the rep $\boldsymbol{A}_m^+$, and *mutatis mutandis* in the rep $\boldsymbol{A}_m^-$.

There is only one family of line groups whose isogonal point groups are $\mathbf{S}_{2n}$, but they are denoted differently for n odd and n even:

$$\mathbf{L}\bar{n}, \quad n = 1, 3, 5, \ldots \qquad \text{and} \qquad \mathbf{L}(\overline{2n}), \quad n = 2, 4, 6, \ldots$$

(see LG). Each of these line groups has a group $\mathbf{L}n$ as its invariant subgroup, so that it can be written:

$$\mathbf{L}n + (\sigma_h C_{2n}|0)\mathbf{L}n, \qquad n = 1, 2, 3, \ldots . \tag{22}$$

Consequently, the general form of its elements is $(C_n^s|t)$ and $(\sigma_h C_{2n} C_n^s|t)$.

Table 10. The reps of the point groups $\mathbf{S}_{2n}$, $n = 1, 2, 3, \ldots$. For α, s, and m see the caption of table 1.

reps	C_n^s	$\sigma_h C_{2n} C_n^s$
$A_m^{\pm}$	$\exp(\mathrm{i}ms\alpha)$	$\pm\exp[\mathrm{i}m(s+1/2)\alpha]$

For $k = 0$ the reps ${}_0\boldsymbol{A}_m^{\pm}$ of these line groups are the same as $\boldsymbol{A}_m^{\pm}$, the reps of the corresponding point groups $\mathbf{S}_{2n}$ (see table 10).

For $0 < |k| < \pi/a$ one has $(\sigma_h C_{2n}|0)(C_n^s|t)(\sigma_h C_{2n}|0)^{-1} = (C_n^s|-t)$, so that

$${}_k\bar{\boldsymbol{A}}_m(\mathbf{L}n) = {}_{-k}\boldsymbol{A}_m(\mathbf{L}n). \tag{23}$$

This means that the two reps of $\mathbf{L}n$, namely, ${}_k\boldsymbol{A}_m (0 < k < \pi/a)$ and ${}_{-k}\boldsymbol{A}_m (-\pi/a < -k < 0)$ induce (as in (8a, b)) one two-dimensional rep ${}_k^{-k}\boldsymbol{E}_m$ of $\mathbf{L}\bar{n}$ or $\mathbf{L}(\overline{2n})$.

Since all the line groups $\mathbf{L}\bar{n}$ and $\mathbf{L}(\overline{2n})$ are symmorphic, it follows that for $k = \pi/a$ their reps (table 11) are constructed as in (11).

Table 11. The reps of the line groups $\mathbf{L}\bar{n}$, $n = 1, 3, 5, \ldots$ and $\mathbf{L}(\overline{2n})$, $n = 2, 4, 6, \ldots$ (see (10), table 10, (8a, b), (23) and (11)). For α, s, m, K see the caption of table 8

$$r/P = \begin{pmatrix} 0 & 1 \\ \exp(\mathrm{i}m\alpha) & 0 \end{pmatrix}.$$

k	reps	$(C_n^s\|t)$	$(\sigma_h C_{2n} C_n^s\|t)$
0	${}_0A_m^{\pm}$	$\exp(\mathrm{i}ms\alpha)$	$\pm\exp[\mathrm{i}m(s+1/2)\alpha]$
$0<k<\pi/a$	${}_k^{-k}E_m$	$\exp(\mathrm{i}ms\alpha)K$	$\exp(\mathrm{i}ms\alpha)PK$
π/a	${}_{\pi/a}A_m^{\pm}$	$(-1)^t\exp(\mathrm{i}ms\alpha)$	$\pm(-1)^t\exp[\mathrm{i}m(s+1/2)\alpha]$

4.3. Reps of the line groups whose isogonal point groups are $\boldsymbol{D}_n$, $n = 1, 2, 3, \ldots$

The point groups $\mathbf{D}_n$, $n = 2, 3, 4, \ldots$ are obtained as semi-direct products of $\mathbf{C}_n$ with $\mathbf{D}_1 = \{E, U\}$, where U is a rotation through π around an axis perpendicular to the z axis (lying in the xy plane):

$$\mathbf{D}_n = \mathbf{C}_n \wedge \mathbf{D}_1 = \mathbf{C}_n + U\mathbf{C}_n, \qquad n = 2, 3, 4, \ldots$$

(cf LG). The elements of $\mathbf{D}_n$ are thus C_n^s and UC_n^s, $n = 1, 2, 3, \ldots$; $s = 0, 1, \ldots, n-1$.

The point groups $\mathbf{D}_n$ and $\mathbf{C}_{nv}$ are isomorphic for the same n. Namely, each group $\mathbf{D}_n$ is determined by its generators C_n and U and the relations between them: $C_n^n = U^2 = E$ and $C_n U = UC_n^{n-1}$; while $\mathbf{C}_{nv}$ is determined by the generators C_n and σ_v, and the analogous relations $C_n^n = \sigma_v^2 = E$ and $C_n\sigma_v = \sigma_v C_n^{n-1}$. Therefore, one has the isomorphism f: $\mathbf{D}_n \to \mathbf{C}_{nv}$ given by $f(C_n) = C_n$ and $f(U) = \sigma_v$. Because of this the groups $\mathbf{D}_n$ and $\mathbf{C}_{nv}$ have the same reps. However, we use somewhat different notation for them since U and σ_v are physically different: U is of R^- type, and σ_v is of R^+

type. Instead of $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{E}_{m,-m}$ used for the reps of $\mathbf{C}_{nv}$, here we make use of $\boldsymbol{A}^+$, $\boldsymbol{A}^-$ and $\boldsymbol{E}_m^{-m}$ respectively (table 12).

Table 12. The reps of the point groups $\mathbf{D}_n$, $n = 1, 2, 3, \ldots$ (see table 3).

reps	C_n^s	UC_n^s
$A_0^\pm$	1	± 1
E_m^{-m}	M	PM
	and only for $n = 2, 4, 6, \ldots$	
$A_{n/2}^\pm$	$(-1)^s$	$\pm(-1)^s$

Note that for $\mathbf{D}_1$ and $\mathbf{D}_2$ there are no two-dimensional reps.

There are two families of line groups which have $\mathbf{D}_n$ as their isogonal point groups. They are (see LG):

(1) $\mathbf{L}n2$, $n = 1, 3, 5, \ldots$ and $\mathbf{L}n22$, $n = 2, 4, 6, \ldots$;

(2) $\mathbf{L}n_p2$, $n = 3, 5, 7, \ldots$ and $\mathbf{L}n_p22$, $n = 2, 4, 6, \ldots$, $p = 1, 2, \ldots, n-1$.

All the members of the first family have $\mathbf{L}n$ as their invariant subgroup, and can be decomposed in the following way: $\mathbf{L}n + (U|0)\mathbf{L}n$. Consequently, the general form of their elements is $(C_n^s|t)$ and $(UC_n^s|t)$, $s = 0, 1, \ldots, n-1$.

For $k = 0$ their reps are given by (10), and for $k = \pi/a$ by (11) (due to the symmorphic property of $\mathbf{L}n2$ and $\mathbf{L}n22$).

For $0 < |k| < \pi/a$ one has to conjugate the reps of $\mathbf{L}n$ (cf table 1) by $(U|0)$ to find out what the conjugate pairs are: $(U|0)(C_n^s|t)(U|0)^{-1} = (C_n^{n-s}|-t)$, which follows from $Ut = -t$ (since U is of R^- type) and $C_nU = UC_n^{n-1}$ (the generator relation for $\mathbf{D}_n$). Consequently,

$$_k\bar{\boldsymbol{A}}_m(\mathbf{L}n) = {}_{-k}\boldsymbol{A}_{-m}(\mathbf{L}n), \tag{24}$$

where $_{-k}A_{-m}(C_n^s|t) = \exp(-ikta)\exp(-ims\alpha)$ (see table 1). The two reps $_k\boldsymbol{A}_m$ and $_{-k}\boldsymbol{A}_{-m}$ of $\mathbf{L}n$ (where $0 < k < \pi/a$ and m is given by (14) or (15)) give rise to one two-dimensional rep $_k^{-k}\boldsymbol{E}_m^{-m}$ of $\mathbf{L}n2$ and $\mathbf{L}n22$ (table 13). Note that for $\mathbf{L}12$ and $\mathbf{L}222$ there are no two-dimensional reps for $k = 0$ and $k = \pi/a$.

Table 13. The reps of the line groups $\mathbf{L}n2$, $n = 1, 3, 5, \ldots$ and $\mathbf{L}n22$, $n = 2, 4, 6, \ldots$ (see (10), table 12, (8*a*, *b*), (24), and (11)). For α, s, M and P see the caption of table 3; for K that of table 8. In the case of $_0\boldsymbol{E}_m^{-m}$ and $_{\pi/a}\boldsymbol{E}_m^{-m}$ the range of m is given by (18*a*, *b*), and for $_k^{-k}\boldsymbol{E}_m^{-m}$ by (14) or (15).

k	reps	$(C_n^s|t)$	$(UC_n^s|t)$
0	$_0A_0^\pm$	1	± 1
0	$_0E_m^{-m}$	M	PM
$0 < k < \pi/a$	$_k^{-k}E_m^{-m}$	KM	PKM
π/a	$_{\pi/a}A_0^\pm$	$(-1)^t$	$\pm(-1)^t$
π/a	$_{\pi/a}E_m^{-m}$	$(-1)^tM$	$(-1)^tPM$
	and only for $n = 2, 4, 6, \ldots$		
0	$_0A_{n/2}^\pm$	$(-1)^s$	$\pm(-1)^s$
π/a	$_{\pi/a}A_{n/2}^\pm$	$(-1)^{s+t}$	$\pm(-1)^{s+t}$

As far as the second family of line groups above is concerned, all its members have $\mathbf{L}n_p$ as their invariant subgroup and can be decomposed as $\mathbf{L}n_p+(U|0)\mathbf{L}n_p$. The general form of their elements is thus $(C_n^s|\mathrm{Fr}(sp/n)+t)$ and $(UC_n^s|\mathrm{Fr}(sp/n)+t)$, $n=2,3,4,\ldots;\ p=1,2,\ldots,n-1$.

For $k=0$ their reps are given by the reps of the corresponding $\mathbf{D}_n$.

For $0<|k|<\pi/a$ we have, in analogy with (24),

$$ {}_k\bar{\boldsymbol{A}}_m(\mathbf{L}n_p)={}_{-k}\boldsymbol{A}_{-m}(\mathbf{L}n_p), \tag{25}$$

where ${}_{-k}A_{-m}(C_n^s|\mathrm{Fr}(sp/n)+t)=\exp\{-\mathrm{i}k[\mathrm{Fr}(sp/n)+t]a\}\exp(-\mathrm{i}ms\alpha)$ (see table 2). Therefore, two reps ${}_k\boldsymbol{A}_m$ and ${}_{-k}\boldsymbol{A}_{-m}$ of $\mathbf{L}n_p$, where $0<k<\pi/a$ and m is given by (14) or (15), induce one two-dimensional rep ${}_k^{-k}\boldsymbol{E}_m^{-m}$ of $\mathbf{L}n_p2$ or $\mathbf{L}n_p22$.

For $k=\pi/a$ one has (see table 2):

$$\begin{aligned}&{}_{\pi/a}A_m(C_n^s|\mathrm{Fr}(sp/n)+t)\\&\qquad=(-1)^{\mathrm{Fr}(sp/n)+t}\exp(\mathrm{i}ms\alpha)=(-1)^{t-\mathrm{Int}(sp/n)}\exp[\mathrm{i}s(m+p/2)\alpha],\end{aligned}$$

since $\mathrm{Fr}(sp/n)=sp/n-\mathrm{Int}(sp/n)$, and

$$\begin{aligned}&{}_{\pi/a}\bar{A}_m(C_n^s|\mathrm{Fr}(sp/n)+t)\\&\qquad=\exp\{-\mathrm{i}\pi[\mathrm{Fr}(sp/n)+t]\}\exp(-\mathrm{i}ms\alpha)\\&\qquad=(-1)^{\mathrm{Int}(sp/n)-t}\exp[-\mathrm{i}s(m+p/2)\alpha]={}_{\pi/a}A_{\bar{m}}(C_n^s|\mathrm{Fr}(sp/n)+t).\end{aligned}$$

In order to calculate $\bar{m}$, i.e. to find which rep is conjugate to that with m, one has to solve the equation

$$\exp[\mathrm{i}s(\bar{m}+p/2)\alpha]=\exp[-\mathrm{i}s(m+p/2)\alpha],$$

giving $s(\bar{m}+m+p)\alpha=0,\ \pm2\pi,\ldots$. Since this must be satisfied for every $s=0,1,\ldots,n-1$, and because $\alpha=2\pi/n$, $-n/2<m\leqslant n/2$ and $0\leqslant p\leqslant n-1$, one obtains $\bar{m}+m+p=\{{}^0_n$, giving finally

$$\bar{m}=\begin{cases}-p-m, & \text{if } -n/2<-p-m\leqslant n/2,\\ n-p-m, & \text{if } -n/2<n-p-m\leqslant n/2.\end{cases}\tag{26}$$

It is easily seen that m in (26) can take on all its values from the interval $(-n/2,n/2]$, but in order to avoid repeated appearance of equivalent reps (see the comment below (8*a*, *b*)), one confines m to half of that interval, i.e. m takes on all the values from the interval $(-p/2,(n-p)/2)$ (see (27) and (28) below), and then $\bar{m}$ takes on the values from $(-n/2,-p/2)$ and $((n-p)/2,n/2]$. The two one-dimensional reps ${}_{\pi/a}\boldsymbol{A}_m$ and ${}_{\pi/a}\boldsymbol{A}_{\bar{m}}$ give rise to one two-dimensional rep ${}_{\pi/a}\boldsymbol{E}_m^{\bar{m}}$.

To find out which reps are self-conjugate, one puts $\bar{m}=m$ in (26) and obtains two equations:

$$m=-p/2,\tag{27}$$

$$m=(n-p)/2.\tag{28}$$

For odd n equation (27) has a solution for even p, and equation (28) for odd p. For even n neither equation has a solution for odd p, while both have one for even p. Table 14 gives the reps of the line groups $\mathbf{L}n_p2$ and $\mathbf{L}n_p22$.

Table 14. The reps of the line groups $\mathbf{L}n_p2$, $n = 3, 5, 7, \ldots$ and $\mathbf{L}n_p22$, $n = 2, 4, 6, \ldots$; $p = 1, 2, \ldots, n-1$ (see (10), table 12, (25), (26), (27), and (28)). For α, s, M, and P see the caption of table 3, for K that of table 8.

$$N = \begin{pmatrix} \exp[\mathrm{i}k\mathrm{Fr}(sp/n)a] & 0 \\ 0 & \exp[-\mathrm{i}k\mathrm{Fr}(sp/n)a] \end{pmatrix},$$

$$H = \begin{pmatrix} \exp(\mathrm{i}sp\alpha/2) & 0 \\ 0 & \exp(-\mathrm{i}sp\alpha/2) \end{pmatrix}, \qquad \beta = (-1)^{\mathrm{Int}(sp/n)};$$

for m in ${}_0\boldsymbol{E}_m^{-m}$ see (18a, b), and in ${}^{-k}_{k}\boldsymbol{E}_m^{-m}$ see (14) or (15); for m and $\tilde{m}$ in ${}_{\pi/a}\boldsymbol{E}_m^{\tilde{m}}$ see (26) and the comment after this equation.

k	reps	$(C_n^s \mid \mathrm{Fr}(sp/n)+t)$	$(UC_n^s \mid \mathrm{Fr}(sp/n)+t)$
0	${}_0A_0^{\pm}$	1	± 1
0	${}_0E_m^{-m}$	M	PM
0 only for n even	${}_0A_{n/2}^{\pm}$	$(-1)^s$	$\pm(-1)^s$
$0<k<\pi/a$	${}^{-k}_{k}E_m^{-m}$	NKM	$PNKM$
π/a	${}_{\pi/a}A_{-p/2}^{\pm}$	$(-1)^t\beta$	$\pm(-1)^t\beta$
π/a	${}_{\pi/a}A_{(n-p)/2}^{\pm}$	$(-1)^{t+s}\beta$	$\pm(-1)^{t+s}\beta$
π/a	${}_{\pi/a}E_m^{\tilde{m}}$	$(-1)^t\beta MH$	$(-1)^t\beta PMH$

Note that the reps ${}_{\pi/a}\boldsymbol{A}_{-p/2}^{\pm}$ and ${}_{\pi/a}\boldsymbol{A}_{(n-p)/2}^{\pm}$ appear only when p and $(n-p)$ respectively are even.

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