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Selection rules for polymers and quasi-one-dimensional crystals: I. Kronecker products for the line groups isogonal to C_n, C_{nv}, C_{nh} and S_{2n}

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Abstract. To derive selection rules for different physical processes occurring in polymers and quasi-one-dimensional solids one has to determine the reduction coefficients for the Kronecker products of the irreducible representations of their symmetry groups, the line groups. This task is accomplished here and the coefficients are tabulated explicitly for all the line groups isogonal to C_n, C_{nv}, C_{nh} and S_{2n} ($n = 1, 2, \ldots$) point groups.

1. Introduction

Recent discoveries of exciting phenomena (Peierls transitions, doping-induced conductivity jumps for up to 20 orders of magnitude, solitons, superconductivity, . . .) in some polymers and quasi-one-dimensional solids have attracted much attention (Barišić *et al* 1980, Bernasconi and Schneider 1981, Devreese *et al* 1979, Seymour 1981). Symmetry properties of such systems thus become worth studying and so the line group theory has been developed. Together with the line groups (Vujičić *et al* 1977) and their unitary irreducible representations (reps) (Božović and Božović 1981, Božović and Vujičić 1981, Božović *et al* 1978) the magnetic line groups (Damnjanović and Vujičić 1982) have been constructed; the applications include electron band structure (Božović *et al* 1981), vibration spectra (Raković *et al* 1982) and phase transition (Damnjanović 1981) studies. The next step should be derivation of selection rules for different physical processes in polymers (optical absorption, electron and neutron scattering, two-phonon Raman and infrared processes, . . .). This task consists largely in reducing the Kronecker products of reps of line groups, and to that the present work is devoted. Thus a gap is filled in the literature in which only a few line groups have been studied (McCubbin 1975), in contrast to the comprehensive studies of the selection rules for the crystallographic space groups (Cracknell *et al* 1979) and point groups (Fackler 1973). In this paper all the line groups isogonal to C_n, C_{nv}, C_{nh} and S_{2n} are considered.

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2. Methods of determining the reduction coefficients for the Kronecker products of reps of line groups

Let us consider a transition of a polymer from the state $|i\rangle$ into the state $|f\rangle$, induced by the perturbation v. If L is the line group of the polymer, the transition is forbidden unless the rep D_f of L is contained in the decomposition (or Clebsch–Gordan) series of the Kronecker product of the reps D_v and D_i. In other words, if

$$D_v \otimes D_i \sim \sum n_{vi,\alpha} D^{\alpha}, \tag{1}$$

where α enumerates all the inequivalent reps of L, then $\langle f|v|i\rangle = 0$ unless $n_{vi,f} \neq 0$. Hence our aim is to determine the reduction (or frequency) coefficients $n_{vi,\alpha}$, for all the reps of line groups. Since the line groups are usually made finite via Born–von Kármán cyclic boundary conditions, one can utilise the character expansion

$$n_{vi,\alpha} = \frac{1}{|L|} \sum_{(R|\tau)\in L} \chi_v(R|\tau)\chi_i(R|\tau)\chi_\alpha(R|\tau)^* \tag{2}$$

where $|L|$ is the order of L and $(R|\tau)$ is an element of L. The required characters are easily deducible from the tables of Božović *et al* (1978) and Božović and Vujičić (1981).

Nice structural features of the line groups (Vujičić *et al* 1977) provide a simpler, recursive method. One first derives $n_{vi,\alpha}$ for the reps of the $\mathrm{L}n_p$ line groups—which is not difficult, since they are all one-dimensional. Every other line group L treated here contains certain $\mathrm{L}n_p$ as an order-two subgroup, and the frequency coefficients of L are then determined recursively (Altmann 1977, Bradley and Cracknell 1972) starting from those of $\mathrm{L}n_p$. The results of § 3 were checked by both methods; some additional tests (e.g. comparing the characters *a posteriori*) were also utilised.

3. Results

In this section for each line group L, where $L = \mathrm{L}n_p$, $\mathrm{L}nm$, $\mathrm{L}nmm$, $\mathrm{L}nc$, $\mathrm{L}ncc$, $\mathrm{L}(2q)_q mc$, $\mathrm{L}n/m$, $\mathrm{L}(2q)_q/m$ or $\mathrm{L}(\overline{2n})$, we give: (a) the character table, introducing the rep symbols and defining the ranges for their quantum numbers, and (b) the table of decompositions of the Kronecker products $D \otimes D'$ for all the inequivalent pairs D, D' of reps of L.

Tables (b) are triangular, in view of $D \otimes D' \sim D' \otimes D$. To simplify the notation, the length unit is chosen to coincide with the repeat length; hence the first Brillouin zone is defined by $k \in (-\pi, \pi]$.

3.1. *The line groups isogonal to C_n*

The line groups isogonal to C_n, $n = 1, 2, \ldots$ are $\mathrm{L}n_p$, $p = 0, 1, \ldots, n-1$. ($\mathrm{L}n_0$ is usually denoted by $\mathrm{L}n$.)

3.2. *The line groups isogonal to C_{nv}*

The line groups isogonal to C_{nv} are $\mathrm{L}nm$ and $\mathrm{L}nc$ for $n = 1, 3, 5, \ldots$ and $\mathrm{L}nmm$, $\mathrm{L}ncc$ and $\mathrm{L}(2q)_q mc$ for $n = 2q = 2, 4, 6, \ldots$. For the non-symmorphic line groups ($\mathrm{L}nc$, $\mathrm{L}ncc$ and $\mathrm{L}(2q)_q mc$) we tabulate the decompositions only for $k + k' \notin (-\pi, \pi]$, because for $k + k' \in (-\pi, \pi]$ they coincide with those of the symmorphic line groups ($\mathrm{L}nm$ and $\mathrm{L}nmm$).

Table 1(a). The characters of the reps of the line groups Ln_p, $n = 1, 2, \ldots, p = 0, 1, \ldots, n-1$. Here $s = 0, 1, \ldots, n-1$, $t = 0, \pm 1, \ldots$, $\alpha = 2\pi/n$, $k \in (-\pi, \pi]$ and m takes on all the integral values from the interval $(-n/2, n/2]$.

Rep	$(C_n^s \mid t + sp/n)$
${}_kA_m$	$\exp(ims\alpha)\exp[ik(t+sp/n)]$

Table 1(b). Decomposition of the Kronecker product $D \otimes D'$ of reps of Ln_p. Notice that for $p = 0$ the index μ becomes independent on $k + k'$.

D \ D'	${}_kA_m$
${}_{k'}A_{m'}$	${}_\kappa A_\mu$

κ and μ depend on $k + k'$ and $m + m'$ as follows:

$k+k'$	$m+m'$	κ	μ
$(-2\pi, -\pi]$	$(-n, -n+p]$	$k+k'+2\pi$	$m+m'-p+2n$
$(-2\pi, -\pi]$	$(-n+p, -n/2+p]$	$k+k'+2\pi$	$m+m'-p+n$
$(-2\pi, -\pi]$	$(-n/2+p, n/2+p]$	$k+k'+2\pi$	$m+m'-p$
$(-2\pi, -\pi]$	$(n/2+p, n]$	$k+k'+2\pi$	$m+m'-p-n$
$(-\pi, \pi]$	$(-n, -n/2]$	$k+k'$	$m+m'+n$
$(-\pi, \pi]$	$(-n/2, n/2]$	$k+k'$	$m+m'$
$(-\pi, \pi]$	$(n/2, n]$	$k+k'$	$m+m'-n$
$(\pi, 2\pi]$	$(-n, -n/2-p]$	$k+k'-2\pi$	$m+m'+p+n$
$(\pi, 2\pi]$	$(-n/2-p, n/2-p]$	$k+k'-2\pi$	$m+m'+p$
$(\pi, 2\pi]$	$(n/2-p, n-p]$	$k+k'-2\pi$	$m+m'+p-n$
$(\pi, 2\pi]$	$(n-p, n]$	$k+k'-2\pi$	$m+m'+p-2n$

Table 2(a). The characters of the reps of the line groups Lnm, $n = 1, 3, \ldots$ and $Lnmm$, $n = 2, 4, \ldots$. For s, t, α and k see the caption of table 1(a); m is an integer such that $1 \leq m \leq (n-1)/2$. The two-dimensional reps appear only for $n \geq 3$.

Rep	$(C_n^s \mid t)$	$(\sigma_v C_n^s \mid t)$
${}_kA_0$	$\exp(ikt)$	$\exp(ikt)$
${}_kB_0$	$\exp(ikt)$	$-\exp(ikt)$
${}_kE_{m,-m}$	$2\cos(ms\alpha)\exp(ikt)$	0
and only for $n = 2q = 2, 4, 6, \ldots$		
${}_kA_q$	$(-1)^s\exp(ikt)$	$(-1)^s\exp(ikt)$
${}_kB_q$	$(-1)^s\exp(ikt)$	$-(-1)^s\exp(ikt)$

Table 2(*b*). Decomposition of the Kronecker product $D \otimes D'$ of reps of L*nm* and L*nmm*. The reps $_kA_q$ and $_kB_q$ appear only in the L*nmm* groups and the heavily framed part of the table corresponds only to these groups.

D \ D'	$_{k'}A_0$	$_{k'}B_0$	$_{k'}E_{m',-m'}$	$_{k'}A_q$	$_{k'}B_q$
$_kA_0$	$_\kappa A_0$				
$_kB_0$	$_\kappa B_0$	$_\kappa A_0$			
$_kE_{m,-m}$	$_\kappa E_{m,-m}$	$_\kappa E_{m,-m}$	(i)		
$_kA_q$	$_\kappa A_q$	$_\kappa B_q$	$_\kappa E_{\delta,-\delta}$	$_\kappa A_0$	
$_kB_q$	$_\kappa B_q$	$_\kappa A_q$	$_\kappa E_{\delta,-\delta}$	$_\kappa B_0$	$_\kappa A_0$

$\delta = q - m'$

$$\kappa = \begin{cases} k + k' + 2\pi & \text{if } k + k' \in (-2\pi, -\pi] \\ k + k' & \text{if } k + k' \in (-\pi, \pi] \\ k + k' - 2\pi & \text{if } k + k' \in (\pi, 2\pi] \end{cases}$$

$$\text{(i)} \quad {}_kE_{m,-m} \otimes {}_{k'}E_{m',-m'} = \begin{cases} {}_\kappa A_0 + {}_\kappa B_0 + {}_\kappa E_{\mu,-\mu} & \text{if } m = m' \neq n/4 \\ {}_\kappa E_{\nu,-\nu} + {}_\kappa E_{\mu,-\mu} & \text{if } m \neq m' \neq (n/2) - m \\ {}_\kappa E_{\nu,-\nu} + {}_\kappa A_q + {}_\kappa B_q, & \text{if } m = q - m' \neq q/2 \text{ (only for } n = 2q = 4, 6, \ldots) \\ {}_\kappa A_0 + {}_\kappa B_0 + {}_\kappa A_q + {}_\kappa B_q & \text{if } m = m' = q/2 \text{ (only for } n = 2q = 4, 8, \ldots) \end{cases}$$

with

$$\mu = \begin{cases} m + m' & \text{if } m + m' \in [2, n/2) \\ n - m - m' & \text{if } m + m' \in (n/2, n-1] \end{cases} \qquad \nu = \begin{cases} m - m' & \text{if } m - m' \in [1, n/2 - 1) \\ -m + m' & \text{if } m - m' \in (-n/2 + 1, -1]. \end{cases}$$

Table 3(*a*). The characters of the reps of the line groups L*nc*, $n = 1, 3, \ldots$ and L*ncc*, $n = 2, 4, \ldots$. For s, t, α and k see the caption of table 1(*a*); m is an integer such that $1 \leq m \leq (n-1)/2$. The two-dimensional reps appear only for $n \geq 3$.

Rep	$(C_n^s \mid t)$	$(\sigma_v C_n^s \mid t + \frac{1}{2})$
$_kA_0$	$\exp(\mathrm{i}kt)$	$\exp[\mathrm{i}k(t + \frac{1}{2})]$
$_kB_0$	$\exp(\mathrm{i}kt)$	$-\exp[\mathrm{i}k(t + \frac{1}{2})]$
$_kE_{m,-m}$	$2\cos(ms\alpha)\exp(\mathrm{i}kt)$	0
and only for $n = 2q = 2, 4, \ldots$		
$_kA_q$	$(-1)^s \exp(\mathrm{i}kt)$	$(-1)^s \exp[\mathrm{i}k(t + \frac{1}{2})]$
$_kB_q$	$(-1)^s \exp(\mathrm{i}kt)$	$-(-1)^s \exp[\mathrm{i}k(t + \frac{1}{2})]$

Table 3(*b*). Decompositions of the Kronecker products of reps of L*nc* and L*ncc*. For $k+k' \in (-\pi, \pi]$ use table 2(*b*) and let $\kappa = k+k'$. For $k+k' \notin (-\pi, \pi]$ the results are given below; δ, μ, ν and (i) as in table 2(*b*). The heavily framed part corresponds only to L*ncc*.

${}_kA_0$	${}_\kappa B_0$				
${}_kB_0$	${}_\kappa A_0$	${}_\kappa B_0$			
${}_kE_{m,-m}$	${}_\kappa E_{m,-m}$	${}_\kappa E_{m,-m}$	(i)		
${}_kA_q$	${}_\kappa B_q$	${}_\kappa A_q$	${}_\kappa E_{\delta,-\delta}$	${}_\kappa B_0$	
${}_kB_q$	${}_\kappa A_q$	${}_\kappa B_q$	${}_\kappa E_{\delta,-\delta}$	${}_\kappa A_0$	${}_\kappa B_0$
D \ D'	${}_{k'}A_0$	${}_{k'}B_0$	${}_{k'}E_{m',-m'}$	${}_{k'}A_q$	${}_{k'}B_q$

$$\kappa = \begin{cases} k+k'+2\pi & \text{if } k+k' \in (-2\pi, -\pi] \\ k+k'-2\pi & \text{if } k+k' \in (\pi, 2\pi] \end{cases}.$$

Table 4(*a*). The characters of the reps of the line groups $L(2q)_q mc$, $q = 1, 2, \ldots$. Here $t = 0, \pm 1, \ldots$, $r = 0, 1, \ldots, q-1$, $k \in (-\pi, \pi]$, $\alpha = \pi/q$ and $m = 1, \ldots, q-1$. In the case of $L2_1mc$ there are no two-dimensional reps.

Reps	$(C_{2q}^{2r}\|t)$	$(C_{2q}^{2r+1}\|t+\frac{1}{2})$	$(\sigma_v C_{2q}^{2r}\|t)$	$(\sigma_v C_{2q}^{2r+1}\|t+\frac{1}{2})$
${}_kA_0$	$\exp(ikt)$	$\exp[ik(t+\frac{1}{2})]$	$\exp(ikt)$	$\exp[ik(t+\frac{1}{2})]$
${}_kB_0$	$\exp(ikt)$	$\exp[ik(t+\frac{1}{2})]$	$-\exp(ikt)$	$-\exp[ik(t+\frac{1}{2})]$
${}_kE_{m,-m}$	$2\cos(2mr\alpha)\exp(ikt)$	$2\cos[m(2r+1)\alpha]\exp[ik(t+\frac{1}{2})]$	0	0
${}_kA_q$	$\exp(ikt)$	$-\exp[ik(t+\frac{1}{2})]$	$\exp(ikt)$	$-\exp[ik(t+\frac{1}{2})]$
${}_kB_q$	$\exp(ikt)$	$-\exp[ik(t+\frac{1}{2})]$	$-\exp(ikt)$	$\exp[ik(t+\frac{1}{2})]$

3.3. The line groups isogonal to C_{nh}

The line groups isogonal to C_{nh} are Ln/m, $n = 1, 2, \ldots$, and $L(2q)_q/m$, $q = 1, 2, \ldots$. Notice that for n odd, Ln/m is also denoted by $L(\bar{2n})$.

3.4. The line groups isogonal to S_{2n}

The line groups isogonal to S_{2n} are $L\bar{n}$, $n = 1, 3, \ldots$ and $L(\overline{2n})$, $n = 2, 4, \ldots$. Analogously to the case of the L*nc*, L*ncc* and $L(2q)_q mc$ line groups, we have to distinguish here whether $m + m' \in (-n/2, n/2]$ or not.

4. Discussions

The selection rules given in § 3 can be interpreted as conservation laws for certain physical observables.

First, the translation symmetry implies that $k_f = k_i + k_v$ if $k_i + k_v \in (-\pi, \pi]$ (a 'normal' process), $k_f = k_i + k_v + Q$ if $k_i + k_v \in (-2\pi, -\pi]$ and $k_f = k_i + k_v - Q$ if

Table 4(*b*). Decomposition of the Kronecker products of reps of $L(2q)_q mc$. For $k+k' \in (-\pi, \pi]$ use table 2(*b*) and let $\kappa = k+k'$. For $k+k' \notin (-\pi, \pi]$ the results are given below.

$_kA_0$	$_\kappa A_q$				
$_kB_0$	$_\kappa B_q$	$_\kappa A_q$			
$_kE_{m,-m}$	$_\kappa E_{\delta,-\delta}$	$_\kappa E_{\delta,-\delta}$	(ii)		
$_kA_q$	$_\kappa A_0$	$_\kappa B_0$	$_\kappa E_{m',-m'}$	$_\kappa A_q$	
$_kB_q$	$_\kappa B_0$	$_\kappa A_0$	$_\kappa E_{m',-m'}$	$_\kappa B_q$	$_\kappa A_q$
D \ D'	$_{k'}A_0$	$_{k'}B_0$	$_{k'}E_{m',-m'}$	$_{k'}A_q$	$_{k'}B_q$

$$\delta = q-m \qquad \text{and} \qquad \kappa = \begin{cases} k+k'+2\pi & \text{if } k+k' \in (-2\pi, -\pi] \\ k+k'-2\pi & \text{if } k+k' \in (\pi, 2\pi] \end{cases}$$

$$\text{(ii)} \quad {}_kE_{m,-m} \otimes {}_{k'}E_{m',-m'} = \begin{cases} {}_\kappa E_{\mu,-\mu} + {}_\kappa A_q + {}_\kappa B_q & \text{if } m = m' \neq q/2 \\ {}_\kappa E_{\mu,-\mu} + {}_\kappa E_{\nu,-\nu} & \text{if } m \neq m' \neq q-m \\ {}_\kappa A_0 + {}_\kappa B_0 + {}_\kappa E_{\nu,-\nu} & \text{if } m = q-m' \neq q/2 \\ {}_\kappa A_0 + {}_\kappa B_0 + {}_\kappa A_q + {}_\kappa B_q & \text{if } m = m' = q/2 \text{ (only for } q = 2, 4, \ldots) \end{cases}$$

with

$$\mu = \begin{cases} q-m-m' & \text{if } m+m' \in [1, q-1] \\ m+m'-q & \text{if } m+m' \in [q+1, 2q-2] \end{cases} \qquad \nu = \begin{cases} q-m'+m & \text{if } m-m' \in [-q+2, -1] \\ q-m+m' & \text{if } m-m' \in [1, q-2]. \end{cases}$$

Table 5(*a*). The characters of the reps of the line groups Ln/m, $n = 1, 2, \ldots$. For s, t, α and m see the caption of table 1(*a*); $k \in (0, \pi]$.

Rep	$(C_n^s \vert t)$	$(\sigma_h C_{2n} C_n^s \vert -t)$
$_0A_m^\pm$	$\exp(ism\alpha)$	$\pm\exp(ims\alpha)$
$^{-k}_{k}E_m$	$2\exp(ims\alpha)\cos(kt)$	0
$_\pi A_m^\pm$	$(-1)^t \exp(ims\alpha)$	$\pm(-1)^t \exp(ims\alpha)$

Table 5(*b*). Decomposition of the Kronecker products of reps of Ln/m.

$_0A_m^\pm$	$_0A_\mu^+$				
$_0A_m^-$	$_0A_\mu^-$	$_0A_\mu^+$			
$^{-k}_{k}E_m$	$^{-k}_{k}E_\mu$	$^{-k}_{k}E_\mu$	(iii)		
$_\pi A_m^+$	$_\pi A_\mu^+$	$_\pi A_\mu^-$	$^{-\lambda}_{\lambda}E_\mu$	$_0A_\mu^+$	
$_\pi A_m^-$	$_\pi A_\mu^-$	$_\pi A_\mu^+$	$^{-\lambda}_{\lambda}E_\mu$	$_0A_\mu^-$	$_0A_\mu^+$
D \ D'	$_0A_{m'}^+$	$_0A_{m'}^-$	$^{-k'}_{k'}E_{m'}$	$_\pi A_{m'}^+$	$_\pi A_{m'}^-$

$\lambda = \pi - k'$

$$\mu = \begin{cases} m + m' + n & \text{if } m + m' \in [-n+1, -n/2] \\ m + m' & \text{if } m + m' \in (-n/2, n/2] \\ m + m' - n & \text{if } m + m' \in (n/2, n] \end{cases}$$

$$\text{(iii)}\quad {}^{-k}_{k}E_m \otimes {}^{-k'}_{k'}E_{m'} = \begin{cases} {}_0A^+_\mu + {}_0A^-_\mu + {}_\pi A^+_\mu + {}_\pi A^-_\mu & \text{if } k = k' = \pi/2 \\ {}_0A^+_\mu + {}_0A^-_\mu + {}^{-\kappa}_{\kappa}E_\mu & \text{if } k = k' \neq \pi/2 \\ {}^{-\gamma}_{\gamma}E_\mu + {}_\pi A^+_\mu + {}_\pi A^-_\mu & \text{if } k = \pi - k' \neq k' \\ {}^{-\gamma}_{\gamma}E_\mu + {}^{-\kappa}_{\kappa}E_\mu & \text{if } k \neq k' \neq \pi - k' \end{cases}$$

with

$$\gamma = \begin{cases} k' - k & \text{if } k - k' \in (-\pi, 0) \\ k - k' & \text{if } k - k' \in (0, \pi) \end{cases} \qquad \kappa = \begin{cases} k + k' & \text{if } k + k' \in (0, \pi) \\ 2\pi - k - k' & \text{if } k + k' \in (\pi, 2\pi). \end{cases}$$

Table 6(*a*). The characters of the reps of the line groups $L(2q)_q/m$, $q = 1, 2, \ldots$. Here $t = 0, \pm 1, \ldots$, $\alpha = \pi/q$, $r = 0, 1, \ldots, q-1$, $m = -q+1, -q+2, \ldots, q$, $w = 1, 2, \ldots, q$ and $k \in (0, \pi]$.

Reps	$(C^{2r}_{2q} \mid t)$	$(C^{2r+1}_{2q} \mid t + \frac{1}{2})$	$(\sigma_h C^{2r}_{2q} \mid -t)$	$(\sigma_h C^{2r+1}_{2q} \mid -t - \frac{1}{2})$
${}_0A^\pm_m$	$\exp(\mathrm{i}2rm\alpha)$	$\exp[\mathrm{i}(2r+1)m\alpha]$	$\pm\exp(\mathrm{i}2rm\alpha)$	$\pm\exp[\mathrm{i}(2r+1)m\alpha]$
${}^{-k}_{k}E_m$	$2\cos(kt)\exp(\mathrm{i}2rm\alpha)$	$2\cos[k(t+\frac{1}{2})]\exp[\mathrm{i}(2r+1)m\alpha]$	0	0
${}_\pi E^{w-q}_w$	$2(-1)^t\exp(\mathrm{i}2rw\alpha)$	0	0	0

Table 6(*b*). Decompositions of the Kronecker products of reps of $L(2q)_q/m$.

${}_0A^+_m$	${}_0A^+_\mu$			
${}_0A^-_m$	${}_0A^-_\mu$	${}_0A^+_\mu$		
${}^{-k}_{k}E_m$	${}^{-k}_{k}E_\mu$	${}^{-k}_{k}E_\mu$	(iv)	
${}_\pi E^{w-q}_w$	${}_\pi E^{\eta-q}_\eta$	${}_\pi E^{\eta-q}_\eta$	(v)	(vi)
D \ D'	${}_0A^+_{m'}$	${}_0A^-_{m'}$	${}^{-k'}_{k'}E_{m'}$	${}_\pi E^{w'-q}_{w'}$

$$\mu = \begin{cases} m + m' + 2q & \text{if } m + m' \in [-2q+2, -q] \\ m + m' & \text{if } m + m' \in [-q+1, q] \\ m + m' - 2q & \text{if } m + m' \in [q+1, 2q] \end{cases}$$

$$\eta = \begin{cases} w + m' + q & \text{if } w + m' \in [-q+2, 0] \\ w + m' & \text{if } w + m' \in [1, q] \\ w + m' - q & \text{if } w + m' \in [q+1, 2q] \end{cases}$$

$$\text{(iv)}\quad {}^{-k}_{k}E_m \otimes {}^{-k'}_{k}E_{m'} = \begin{cases} {}_0A^+_\mu + {}_0A^-_\mu + {}_\pi E^{\rho-q}_\rho & \text{if } k = k' = \pi/2 \\ {}_0A^+_\mu + {}_0A^-_\mu + {}^{-\kappa}_{\kappa}E_\mu & \text{if } k = k' \neq \pi/2 \\ {}^{-\gamma}_{\gamma}E_\mu + {}_\pi E^{\rho-q}_\rho & \text{if } k = \pi - k' \neq k' \\ {}^{-\gamma}_{\gamma}E_\mu + {}^{-\kappa}_{\kappa}E_\mu & \text{if } k \neq k' \neq \pi - k \end{cases}$$

with

$$\gamma=\begin{cases} k'-k & \text{if } k-k'\in(-\pi,0) \\ k-k' & \text{if } k-k'\in(0,\pi) \end{cases} \qquad \kappa=\begin{cases} k+k' & \text{if } k+k'\in(0,\pi) \\ 2\pi-k-k' & \text{if } k+k'\in(\pi.\,2\pi) \end{cases}$$

$$\rho=\begin{cases} m+m'+2q & \text{if } m+m'\in[-2q+2,-q] \\ m+m'+q & \text{if } m+m'\in[-q+1,0] \\ m+m' & \text{if } m+m'\in[1,q] \\ m+m'-q & \text{if } m+m'\in[q+1,2q]. \end{cases}$$

(v) ${}_{\pi}E_{w}^{w-q}\otimes{}^{-k'}_{k'}E_{m'}={}^{-\lambda}_{\lambda}E_{\beta}+{}^{-\lambda}_{\lambda}E_{\beta-q}$

where $\lambda=\pi-k'$

$$\beta=\begin{cases} w+m'+q & \text{if } w+m'\in[-q+2,0] \\ w+m' & \text{if } w+m'\in[1,q] \\ w+m'-q & \text{if } w+m'\in[q+1,2q]. \end{cases}$$

(vi) ${}_{\pi}E_{w}^{w-q}\otimes{}_{\pi}E_{w'}^{w'-q}={}_{0}A_{\tau}^{+}+{}_{0}A_{\tau}^{-}+{}_{0}A_{\tau-q}^{+}+{}_{0}A_{\tau-q}^{-}$

where $\tau=\begin{cases} w+w' & \text{if } w+w'\in[2,q] \\ w+w'-q & \text{if } w+w'\in[q+1,2q]. \end{cases}$

Table 7(*a*). The characters of the reps of the line groups $L\bar{n}$, $n=1,3,\ldots$ and $L(\overline{2n})$, $n=2,4,\ldots$. For s, t, α and m see the caption of table 1(a); $k\in(0,\pi]$.

Reps	$(C_n^s\|t)$	$(\sigma_h C_{2n} C_n^s\|-t)$
${}_{0}A_m^{\pm}$	$\exp(ims\alpha)$	$\pm\exp[im(s+\frac{1}{2})\alpha]$
${}^{-k}_{k}E_m$	$2\cos(kt)\exp(ims\alpha)$	0
${}_{\pi}A_m^{\pm}$	$(-1)^t\exp(ims\alpha)$	$\pm(-1)^t\exp[im(s+\frac{1}{2})\alpha]$

Table 7(*b*). Decompositions of the Kronecker products of reps of $L\bar{n}$ ($n$odd) and $L(\overline{2n})$ (n even). The results for $m+m'\in(-n/2,n/2]$ differ from those for $m+m'\notin(-n/2,n/2]$ and hence each case is discussed separately. Here $\lambda=\pi-k'$ and (iii) is given in table 5(b).

For $m+m'\in(-n/2,n/2]$

${}_{0}A_m^{+}$	${}_{0}A_{\mu}^{+}$				
${}_{0}A_m^{-}$	${}_{0}A_{\mu}^{-}$	${}_{0}A_{\mu}^{+}$			
${}^{-k}_{k}E_m$	${}^{-k}_{k}E_{\mu}$	${}^{-k}_{k}E_{\mu}$	(iii)		
${}_{\pi}A_m^{+}$	${}_{\pi}A_{\mu}^{+}$	${}_{\pi}A_{\mu}^{-}$	${}^{-\lambda}_{\lambda}E_{\mu}$	${}_{0}A_{\mu}^{+}$	
${}_{\pi}A_m^{-}$	${}_{\pi}A_{\mu}^{-}$	${}_{\pi}A_{\mu}^{+}$	${}^{-\lambda}_{\lambda}E_{\mu}$	${}_{0}A_{\mu}^{-}$	${}_{0}A_{\mu}^{+}$
D \\ D'	${}_{0}A_{m'}^{+}$	${}_{0}A_{m'}^{-}$	${}^{-k}_{k}E_{m'}$	${}_{\pi}A_{m'}^{+}$	${}_{\pi}A_{m'}^{-}$

where $\mu=m+m'$.

For $m+m' \notin (-n/2, n/2]$

${}_0A^+_m$	${}_0A^-_\mu$				
${}_0A^-_m$	${}_0A^+_\mu$	${}_0A^-_\mu$			
${}^{-k}_{k}E_m$	${}^{-k}_{k}E_\mu$	${}^{-k}_{k}E_\mu$	(iii)		
${}_\pi A^+_m$	${}_\pi A^-_\mu$	${}_\pi A^+_\mu$	${}^{-\lambda}_{\lambda}E_\mu$	${}_0A^-_\mu$	
${}_\pi A^-_m$	${}_\pi A^+_\mu$	${}_\pi A^-_\mu$	${}^{-\lambda}_{\lambda}E_\mu$	${}_0A^+_\mu$	${}_0A^-_\mu$
D / D'	${}_0A^+_{m'}$	${}_0A^-_{m'}$	${}^{-k}_{k}E_{m'}$	${}_\pi A^+_{m'}$	${}_\pi A^-_{m'}$

where

$$\mu = \begin{cases} m+m'+n & \text{if } m+m' \in (-n, -n/2] \\ m+m'-n & \text{if } m+m' \in (n/2, n]. \end{cases}$$

$k_i + k_v \in (\pi, 2\pi]$ ('Umklapp' processes), where $Q = 2\pi$. Since the reps d_k, d_{k+Q} and d_{k-Q} are all equivalent, the quasi-momentum $p = \hbar k$ is conserved in either case; briefly,

$$k_i \doteq k_f + k_v \tag{3}$$

where $\doteq$ means 'equal modulo Q'. The result is valid also for the line groups isogonal to either C_n or C_{nv}. However, the remaining ones contain elements which convert k into $-k$, and their reps are in general labelled by pairs $\{k, -k\}$, so that (3) has to be modified in that case.

Let $|i\rangle$, $|f\rangle$ and v be labelled by $\{k_i, -k_i\}$, $\{k_f, -k_f\}$ and $\{k_v, -k_v\}$, respectively; $\langle i|v|f\rangle = 0$ unless

$$k_f \doteq k_i + k_v \qquad \text{or} \qquad k_f \doteq k_i - k_v. \tag{4}$$

Let us turn now to C_n, the rotation through $2\pi/n$ around the chain axis. The corresponding quantum number is m, an integer from $(-n/2, n/2]$, and the selection rule reads

$$m_f \doteq m_i + m_v \tag{5}$$

where $\doteq$ stands for 'equal modulo n'. Hence the quasi-angular momentum $l = \hbar m$ is conserved; this conclusion is also valid for all the line groups which contain C_n as a subgroup.

However, in the Ln_p line groups rotations are coupled to translations and reps are labelled by pairs $\{k, m\}$; $\langle i|v|f\rangle \neq 0$ requires that

$$k_f = k_i + k_v \qquad \text{and} \qquad m_f \doteq m_i + m_v \tag{6}$$

for normal processes, or

$$k_f = k_i + k_v + Q \qquad \text{and} \qquad m_f \doteq m_i + m_v + p \tag{7a}$$

or

$$k_f = k_i + k_v - Q \qquad \text{and} \qquad m_f \doteq m_i + m_v - p \tag{7b}$$

for Umklapp processes ($\doteq$ as in (5)). Non-conservation of m in (7a, b) is due to the fact that for $p \neq 0$, $(C_n|0)$ does not belong to Ln_p.

Finally, let us consider the parity with respect to the vertical mirror plane σ_v, distinguished by the symbols A (even reps) and B (odd reps). In the case of the Lnm, Lnmm and L$(2q)_q mc$ line groups which contain $(\sigma_v|0)$ this parity is strictly conserved; for Lnc and Lncc, $(\sigma_v|0) \notin L$ and in Umklapp processes the parity is reversed. Analogously, the parity with respect to the horizontal mirror plane σ_h (indicated by the superscript $\pm$) is conserved in the Ln/m and L$(2q)_q/m$ groups for which $(\sigma_h|0) \in L$, while it is reversed if $m_i + m_v \notin (-n/2, n/2]$ in the L$(\overline{2n})$ groups which do not contain $(\sigma_h|0)$.

Few additional remarks might be of interest. First, for a particular physical process v is specified and hence its rep D_v can be determined; the selection rules may then become even more restrictive. For example, in the case of direct optical absorption one has (Božović *et al* 1981) $k_v = 0$ and $m_v = 0, \pm 1$ so that the rules (6, 7a, b) become

$$\Delta k \equiv k_f - k_i = 0 \qquad \text{and} \qquad \Delta m \equiv m_f - m_i \doteq 0, \pm 1.$$

For special directions of incidence and polarisations of light further specifications are obtained, relevant for understanding dichroic effects in polymers. Next, some additional restrictions may be obtained for degenerate reps *via* the Wigner-Eckart theorem.

Notice also that the $k = 0$ reps of a line group L coincide with the reps of the point group P isogonal to L; our tables thus contain the selection rules for the axial point groups, too. Finally, the Kronecker product is distributive with respect to direct matrix summation and hence the tables of § 3 enable easy reduction of multiple Kronecker products like $D \otimes D' \otimes D''$, etc.

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