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Selection rules for vibronic coupling in quasi-one-dimensional solids III: staggered molecular stacks

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Abstract. Vibronic instabilities in conducting polymers and quasi-one-dimensional metals are studied. For all the line groups that contain glide planes, the symmetrized Kronecker squares of irreducible representations are decomposed into irreducible constituents. The derivation of the selection rules for linear-vibronic-coupling matrix elements is thus completed for all the line groups.

1. Introduction

Organic compounds such as TMTSF (bis-tetramethyl-tetraselenafulvalene), NMP (*N*-methylphenazinium), HMTTF (hexamethylene tetrathiafulvalene), TTT (tetrathiatetracene), TSeT (tetraselenatetracene), and the like frequently crystallize in a peculiar form of staggered molecular stacks. Such compounds have attracted worldwide attention from physicists and chemists (Miller 1982, Monceau 1985, Kamimura 1985, Kuzmany *et al* 1985, Skotheim 1986), when it was discovered that $(\text{TMTSF})_2\text{ClO}_4$ becomes superconducting with $T_c = 1.4$ K (at pressures above 7 kbar). That was quite unexpected, since neither of the constituent elements is superconducting itself; indeed, it was the first organic superconductor discovered. Before long, a few other related compounds such as $(\text{HMTTF})_2\text{ClO}_4$ were synthesized, and some of these were found to be superconducting at normal pressure and with critical temperatures up to 13 K so far.

Although many details of the underlying physics remain to be clarified, it seems certain that one of the key ingredients is the reduced dimensionality of the electronic subsystem. In such materials, certain topological effects—e.g. the Peierls (or charge-density-wave) instability, or the spin-density-wave instability—are generally expected (Peierls 1955) to occur. To study these systematically, one needs to know the selection rules for the matrix elements of the relevant scattering process—e.g. the linear electron-phonon coupling matrix elements in the case of vibronic instabilities. Technically, these are derived by finding all the irreducible components of the symmetrized Kronecker squares (SKS) of all the irreducible corepresentations of the line groups. Precisely that task has been accomplished in this series of papers (Božović and Božović

1989, 1990, to be referred to as I and II, respectively); the present paper completes it by considering all the line groups that contain a glide plane, i.e. the groups Lnc ($n=1, 2, \dots$) and $Lncc$ ($n=2, 4, \dots$) isogonal to C_{nv} , $L\bar{n}c$ ($n=1, 2, \dots$) and $L(\bar{2}n)2c$ ($n=2, 4, \dots$) isogonal to D_{nd} , and $L(2n)2c$ ($n=1, 3, \dots$) and Ln/mcc ($n=2, 4, \dots$) isogonal to D_{nh} .

The paper is organized as follows. In section 2, we introduce the notation to be utilized in the tables; in section 3 the tables of the irreducible components of the sks of the irreducible corepresentations of the groups under study are given; in section 4 some examples are presented, and in section 5 we summarize our conclusions. For the reader's convenience, the character tables of the corepresentations of the groups under study are given in the appendix.

2. Notation

Let us define some of the notation which we shall use:

$A(B)$: one-dimensional irreducible representation, irrep, of a line group L , even (odd) with respect to the vertical mirror plane;

E : a two-dimensional irrep of L ;

G : a four-dimensional irrep of L ;

(D, D^*) : a pair of complex-conjugate irreps, a corepresentation of L ;

$\hbar k$: quasi-momentum; we choose $\hbar = 1$ and the translation period $a = 1$ so that $0 < k < \pi$;

$\hbar m$: quasi-angular momentum; $m = 1, 2, \dots, (n-2)/2$ for n even and $m = 1, 2, \dots, (n-1)/2$ for n odd, where n is the order of the screw axis.

In tables 1-3 we also utilize the following abbreviations:

$$r = 2k \quad t = 2\pi - 2k \quad w = 2m \quad v = 2m - n.$$

3. Tables of irreducible components of the symmetrized Kronecker squares of corepresentations of all the line groups that contain a glide plane

Since the sks of an one-dimensional corepresentation is one-dimensional (and hence irreducible) itself, in the following tables 1-3 we list the irreducible constituents of the sks of higher- (two or four) dimensional corepresentations only.

4. Examples

Let us illustrate how these tables can be utilized by considering a staggered stack of identical diatomic molecules shown in figure 1. A similar model has already been described in II; the difference is that the neighbouring molecules were at right angles with respect to one another, and the overall line group symmetry was $L4_2/mcm$ there; here the angle is assumed to be different from $0, \pm\pi/2$, which reduces the symmetry onto $L2/mcc$. Let us suppose that each atom contributes one relevant atomic orbital of the $l=0$ type (i.e. s, p, d_z , etc) and let t_1 and t_2 denote the intra- and inter-molecular transfer integrals as indicated in figure 1. The tight-binding electronic energy bands are

$$\begin{aligned} E(kA0) &= 2t_1 + 2t_2 \cos k & E(kB0) &= 2t_1 - 2t_2 \cos k \\ E(kA1) &= -2t_1 + 2t_2 \cos k & E(kB1) &= -2t_1 - 2t_2 \cos k. \end{aligned}$$

Table 1. SKS of corepresentations of the line groups Lnc ($n = 1, 3, \dots$) and Lnc_c ($n = 2, 4, \dots$).

D		$[D^2] - (0A0)$	
$(0Em)$	$m < q/2$	$(0Ew)$	
	$m = q/2^\ddagger$	$(0Aq) + (0Bq)$	
	$m > q/2$	$(0Ev)$	
$(kA0, -kA0)$	$k < \pi/2$	$(rA0, -rA0)$	
	$k = \pi/2$	$(\pi A0, \pi B0)$	
	$k > \pi/2$	$(tB0, -tB0)$	
$(kB0, -kB0)$	$k < \pi/2$	$(rA0, -rA0)$	
	$k = \pi/2$	$(\pi A0, \pi B0)$	
	$k > \pi/2$	$(tB0, -tB0)$	
$(kEm, -kEm)$	$k < \pi/2$	$m < q/2$	$(rEw, -rEw) + (rA0, -rA0) + (0Ew) + (0B0)$
		$m = q/2^\ddagger$	$(rAq, -rAq) + (rBq, -rBq) + (rA0, -rA0) + (0Aq) + (0Bq) + (0B0)$
		$m > q/2$	$(rEv, -rEv) + (rA0, -rA0) + (0Ev) + (0B0)$
	$k = \pi/2$	$m < q/2$	$(\pi Ew, \pi Ew) + (\pi A0, \pi B0) + (0Ew) + (0B0)$
		$m = q/2^\ddagger$	$2(\pi A0, \pi B0) + (\pi Aq, \pi Bq) + (0Aq) + (0Bq) + (0B0)$
		$m > q/2$	$(\pi Ev, \pi Ev) + (\pi A0, \pi B0) + (0Ev) + (0B0)$
	$k > \pi/2$	$m < q/2$	$(tEw, -tEw) + (tB0, -tB0) + (0Ew) + (0B0)$
		$m = q/2^\ddagger$	$(tAq, -tAq) + (tB2, -tB2) + (tB0, -tB0) + (0Aq) + (0B0)$
		$m > q/2$	$(tEv, -tEv) + (tB0, -tB0) + (0Ev) + (0B0)$
$(kAq, -kAq)$	$k < \pi/2$	$(rA0, -rA0)$	
	$k = \pi/2$	$(\pi A0, \pi B0)$	
	$k > \pi/2$	$(tB0, -tB0)$	
$(kBq, -kBq)^\dagger$	$k < \pi/2$	$(rA0, -rA0)$	
	$k = \pi/2$	$(\pi A0, \pi B0)$	
	$k > \pi/2$	$(tB0, -tB0)$	
$(\pi A0, \pi B0)$		$2(0B0)$	
$(\pi Em, \pi Em)$	$m < q/2$	$3(0Ew) + 3(0B0)$	
	$m = q/2^\ddagger$	$3(0Aq) + 3(0Bq) + 3(0B0)$	
	$m > q/2$	$3(0Ev) + 3(0B0)$	
$(\pi Aq, \pi Bq)^\dagger$		$2(0B0)$	

† Only for $n = 2q = 2, 4, \dots$

‡ Only for $q = 2, 4, \dots$

For simplicity, let us assume that $t_1 < 0$, $t_2 < 0$ and $|t_2| > |t_1|$ to avoid band overlapping; in that case there is no band degeneracy except at $k = \pi$ where they cross pairwise: $A0$ merges with $B0$, and $A1$ with $B1$, respectively, at $k = \pi/2$. In terms of the classification given in Božović (1984), they form two semiloop bandshapes. In what follows we will consider the cases when each molecule contributes one electron so that the lowest $A0$ band is half-filled, and when each molecule contributes two electrons so that it is completely occupied.

Case 1. Here the Fermi level states belong to

$$D = (\pi/2A0) + (-\pi/2A0) = (\pi/2EA0).$$

Table 2. SKS of corepresentations of the line groups $L\bar{n}c$ ($n=1, 3, \dots$) and $L(\overline{2n})2c$ ($n=2, 4, \dots$).

D		$[D^2]-(0A0)$
$(0Em\pm)$	$m < q/2$ $m = q/2\ddagger$ $m > q/2$	$(0Ew+)$ $(0Eq+)$ $(0Ev+)$
$(0Eq)$		$(0A0+) + (0B0+)$
$(kEA0)$	$k < \pi/2$ $k = \pi/2$ $k > \pi/2$	$(rEA0)$ $(\pi E0)$ $(tEB0)$
$(kEB0)$	$k < \pi/2$ $k = \pi/2$ $k > \pi/2$	$(rEA0)$ $(\pi E0)$ $(tEB0)$
(kGm)	$k < \pi/2$ $m < q/2$ $m = q/2\ddagger$ $m > q/2$ $k = \pi/2$ $m < q/2$ $m = q/2\ddagger$ $m > q/2$ $k > \pi/2$ $m < q/2$ $m = q/2\ddagger$ $m > q/2$	$(rGw) + (rEA0) + (0Ew+) + (0B0-)$ $2(rEq) + (rEA0) + (0Eq) + (0B0-)$ $(rGv) + (rEA0) + (0Ev+) + (0B0-)$ $(\pi Ew+, \pi Ew-) + (\pi E0) + (0Ew+) + (0B0-)$ $(\pi Aq+, \pi Bq+) + (\pi Aq-, \pi Bq-) + (\pi E0) + (0Eq) + (0B0-)$ $(\pi Ev+, \pi Ev-) + (\pi E0) + (0Ev-) + (0B0-)$ $(tGw) + (tEB0) + (0Ew+) + (0A0-)$ $2(tEq) + (tEB0) + (0Eq) + (0A0-)$ $(tGv) + (tEB0) + (0Ev+) + (0A0-)$
$(\pi E0)$		$(0B0+) + (0B0-)$
$(\pi Em+, \pi Em-)$	$m < q/2$ $m = q/2\ddagger$ $m > q/2$	$2(0Ew+) + (0Ew-) + 2(0B0+) + (0B0-)$ $3(0Eq) + 2(0B0+) + (0B0-)$ $2(0Ev+) + (0Ev-) + 2(0B0+) + (0B0-)$
$(\pi Aq+, \pi Bq+)\dagger$		$2(0B0+)$

† Only for $n = 2q = 2, 4, \dots$

‡ Only for $q = 2, 4, \dots$

From table 3, entry $(kEA0)$, case $k = \pi/2$, we find that

$$[\pi/2EA_0^2] = (\pi EA0) + (0A0+).$$

(Notice the identity corepresentation appears in every $[D^2]$; it was omitted from tables 1-3 for brevity.)

Now, we have to construct the symmetry adapted displacement modes that transform according to the two corepresentations, $(0A0+)$ and $(\pi EA0)$, for which we can utilize the method expounded in Božović and Delhalle (1984). The resulting displacement modes are shown in figures 2 and 3. In the case of $(\pi EA0)$, the modes are pairwise-degenerate, implying the existence of a vibronic instability with a complex order parameter. The breathing mode in figure 2 is transverse optic, and it is of high frequency since it involves bond stretching. The modes in figures 3(a) are transverse and distortive; those in figure 3(b) are displacive and longitudinal and they are analogous to the customary Peierls modes.

Table 3. SKS of corepresentations of the line groups $L(\overline{2n})2c$ ($n = 1, 3, \dots$) and L_n/mcc ($n = 2, 4, \dots$).

D		$[D^2] - (0A0+)$	
$(0Em\pm)$	$m < q/2$	$(0Ew+)$	
	$m = q/2\ddagger$	$(0Aq+) + (0Bq+)$	
	$m > q/2$	$(0Ev+)$	
$(kEA0)$	$k < \pi/2$	$(rEA0)$	
	$k = \pi/2$	$(\pi E0)$	
	$k > \pi/2$	$(tEB0)$	
$(kEB0)$	$k < \pi/2$	$(rEA0)$	
	$k = \pi/2$	$(\pi E0)$	
	$k > \pi/2$	$(tEB0)$	
(kGm)	$k < \pi/2$	$m < q/2$	$(rGw) + (rEA0) + (0Ew+) + (0B0-)$
		$m = q/2\ddagger$	$(rEAq) + (rEBq) + (rEA0) + (0Aq+) + (0Bq+) + (0B0-)$
	$k = \pi/2$	$m > q/2$	$(rGv) + (rEA0) + (0Ev+) + (0B0-)$
		$m < q/2$	$(\pi Ew+, \pi Ew-) + (\pi E0) + (0Ew+) + (0B0-)$
		$m = q/2\ddagger$	$2(\pi Eq) + (\pi E0) + (0Aq+) + (0Bq+) + (0B0-)$
	$k > \pi/2$	$m > q/2$	$(\pi Ev+, \pi Ev-) + (\pi E0) + (0Ev+) + (0B0-)$
		$m < q/2$	$(tGw) + (tEB0) + (0Ew+) + (0A0-)$
		$m = q/2\ddagger$	$(tEAq) + (tEBq) + (tEB0) + (0Aq+) + (0Bq+) + (0A0-)$
		$m > q/2$	$(tGv) + (tEB0) + (0Ev+) + (0A0-)$
$(kEAq)\dagger$	$k < \pi/2$	$(tEA0)$	
	$k = \pi/2$	$(\pi E0)$	
	$k > \pi/2$	$(tEBq)$	
$(kEBq)\dagger$	$k < \pi/2$	$(tEA0)$	
	$k = \pi/2$	$(\pi E0)$	
	$k > \pi/2$	$(tEB0)$	
$(\pi E0)$		$(0B0+) + (0B0-)$	
$(\pi Em+, \pi Em-)\ddagger$	$m < q/2$	$2(0Ew+) + (0Ew-) + 2(0B0+) + (0B0-)$	
	$m = q/2\ddagger$	$2(0Aq+) + 2(0Bq+) + (0Aq-) + (0Bq-) + 2(0B0+) + (0B0-)$	
	$m > q/2$	$2(0Ev+) + (0Ev-) + 2(0B0+) + (0B0-)$	
$(\pi Eq)\dagger$		$2(0B0+)$	

† Only for $n = 2q = 2, 4, \dots$

‡ Only for $q = 2, 4, \dots$

Case 2. Here the states at the Fermi level transform according to

$$D = (\pi E0).$$

From table 5, entry $(\pi/2E0)$, one finds that

$$[\pi E0^2] = (0B0+) + (0B0-) + (0A0+).$$

None of these vibronically active modes are degenerate. Of these, the $(0B0+)$ mode shown in figure 4(a) is transverse and distortive, and that in figure 4(b) is transverse

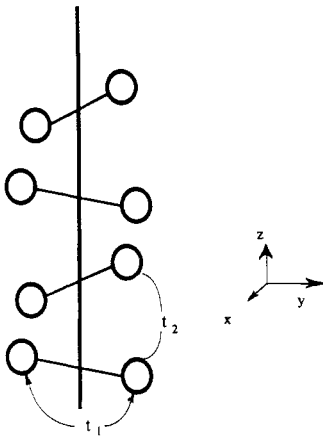


Figure 1. A staggered stack of identical diatomic molecules.

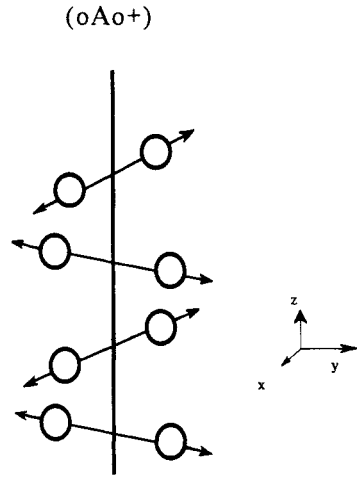


Figure 2. The displacement mode which transforms according to the representation (0A₀⁺).

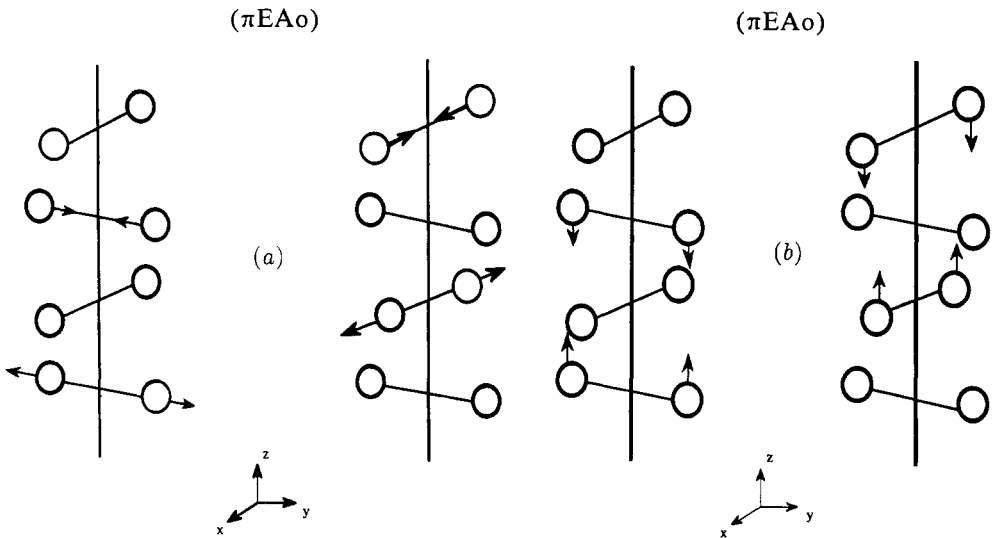


Figure 3. The displacement modes which transforms according to the representation (πEA₀).

and displacive; the former is the low-frequency vibration mode which could be expected to dominate the instability. The (0B₀⁻) mode shown in figure 5 is displacive and longitudinal.

5. Conclusions and discussion

Having completed the derivation of the line-group selection rules for vibronic coupling, we are now in a position to compare the present results with those of I and II, to draw some parallels, and point out some specific consequences of the presence or absence of particular symmetry elements.

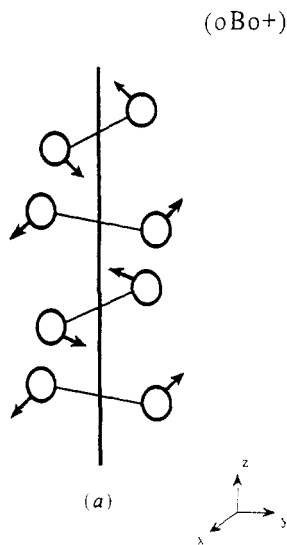


Figure 4. The (oBo+) modes.

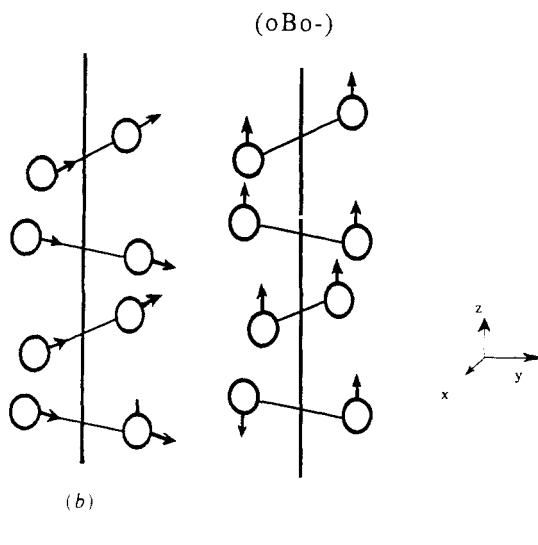


Figure 5. The (oBo-) mode.

The main issue, of course, is conservation of certain quantum numbers. The quasi-momentum $\hbar k$ is found to be conserved without restrictions. The same is true for the quasi-angular momentum, unless the line group under consideration contains a screw axis. And even in the latter case, it is strictly conserved in all 'normal' scattering processes, in which $2k < \pi$ (the Brillouin zone edge). In the case of so-called 'Umklapp' processes, with $2k \geq \pi$, it jumps according to the rule $(k, m) \rightarrow (k + 2\pi, m + p)$, as a result of coupling of rotational and translational symmetry operations, as explained in II. A similar statement can be made for the parity with respect to a vertical mirror plane—it is strictly conserved without restrictions unless one deals with a glide plane, and in that case the parity is reversed in 'Umklapp' processes while it is conserved in 'normal' processes. Even with that little complication in the case of 'Umklapp' processes in non-symmorphic line groups, the conservation or modification rules for these additional quantum numbers are simple and provide a mnemonically easy alternative to actually constructing the symmetrized Kronecker squares, and decomposing them, etc. With the help of these rules one should be able, for example, to easily and rigorously determine all the vibronically active displacements of a quasi-one-dimensional metal, as has been illustrated on several examples in this series of papers. Without them, it is indeed easy to miss some of the relevant modes and arrive at essentially wrong conclusions concerning the stability of the physical system considered; for an assessment and critique of several such cases see Božović (1985, 1986).

The next relevant issue is that of the dimensionality of the order parameter involved. As already pointed out in I and II, if the line group is rich enough to have a four-dimensional corepresentation, and if the electronic band structure of the polymer considered is such that the Fermi level falls in a band labelled with such a corepresentation, it may happen that there are four degenerate vibrational modes that drive (or dominate) the vibronic instability. Such a situation has not been clearly identified so far; there are some indications that it could be occurring in TaTi₄ (Sherwin *et al* 1986). Of focal interest in such cases is the possibility (Božović 1984) that two independent Goldstone modes could occur.

Finally, this series makes the task of providing a constructive proof of the polymer (i.e. the line group) analogue of the Jahn-Teller theorem (Jahn and Teller 1937, Peierls 1955) much easier. It would be sufficient to explicitly construct the vibrational symmetry-adapted bases for all the inequivalent graphs (sets of points generated by the line group) of all the line groups (cf, e.g., Božović and Delhalle 1984, Koch and Seelig 1987), and to identify in each case at least one non-trivial vibronically active mode. Work along these lines is in progress.

Appendix

Listed below are the characters of all the irreducible corepresentations of the line groups under study (i.e. all that contain a glide plane). The characters are listed here only for the necessary elements (coset representatives) since that is sufficient to identify the corepresentation. In these tables, $s = 0, 1, \dots, n-1$; $t = 0, \pm 1, \pm 2, \dots$, and $\alpha = 2\pi/n$.

Table 4. The characters of irreducible corepresentations of the line groups Lnc ($n = 1, 3, \dots$) and Lnc ($n = 2, 4, \dots$).

D	$(C_n t)$	$(\sigma_v \frac{1}{2})$
(0A0)	1	1
(0B0)	1	-1
(0Em)	$2 \cos(ms\alpha)$	0
(0Aq) [†]	$(-1)^s$	-1
(0Bq) [†]	$(-1)^s$	1
(kA0, -kA0)	$2 \cos(kt)$	$2 \cos(k/2)$
(kB0, -kB0)	$2 \cos(kt)$	$-2 \cos(k/2)$
(kEm, -kEm)	$4 \cos(ms\alpha) \cos(kt)$	0
(kAq, -kAq) [†]	$2(-1)^s \cos(kt)$	$2 \cos(k/2)$
(kBq, -kBq) [†]	$2(-1)^s \cos(kt)$	$-2 \cos(k/2)$
(π A0, π B0) [†]	$2(-1)^t$	0
(π Em, π Em)	$4(-1)^t \cos(ms\alpha)$	0
(π Aq, π Bq) [†]	$2(-1)^{s+t}$	0

[†] Only for $n = 2q = 2, 4, \dots$

Table 5. The characters of irreducible corepresentations of the line groups $L\bar{n}c$ ($n = 1, 3, \dots$) and $L(\bar{2}n)2c$ ($n = 2, 4, \dots$).

D	$(C_n^2 t)$	$\sigma_v 1/2)$	$(U_d 0)$	$(\sigma_v U_d 0)$
(0A0 \pm)	1	1	± 1	± 1
(0B0 \pm)	1	-1	± 1	± 1
(0Em \pm)	$2 \cos(ms\alpha)$	0	0	$\pm 2 \cos(m\alpha/2)$
(0Eq) [†]	$2(-1)^s$	0	0	0
(kEA0)	$2 \cos(kt)$	$2 \cos(k/2)$	0	0
(kEB0)	$2 \cos(kt)$	$-2 \cos(k/2)$	0	0
(kGm)	$4 \cos(ms\alpha) \cos(kt)$	0	0	0
(kEAq, kEBq) [†]	$4(-1)^s \cos(kt)$	0	0	0
(π E0)	$2(-1)^t$	0	0	0
(π Em \pm , π Em \pm)	$4(-1)^t \cos(ms\alpha)$	0	0	0
(π Aq \pm , π Bq \pm) [†]	$2(-1)^{s+t}$	0	± 2	0

[†] Only for $q = 2, 4, \dots$

Table 6. The characters of irreducible corepresentations of the line groups $L(2n)2c$ ($n = 1, 3, \dots$) and Ln/mcc ($n = 2, 4, \dots$).

D	$(C_n^s t)$	$(\sigma_v \frac{1}{2})$	$(\sigma_h 0)$
$(0A0\pm)$	1	1	± 1
$(0B0\pm)$	1	-1	± 1
$(0Em\pm)$	$2 \cos(m\alpha)$	0	± 2
$(0Aq\pm)^\dagger$	$(-1)^q$	1	± 1
$(0Bq\pm)^\dagger$	1	-1	± 1
$(kEA0)$	$2 \cos(kt)$	$2 \cos(k/2)$	0
$(kEB0)$	$2 \cos(kt)$	$-2 \cos(k/2)$	0
(kGm)	$4 \cos(m\alpha) \cos(kt)$	0	0
$(kEAq)^\dagger$	$2 \cos(kt)$	$2 \cos(k/2)$	0
$(kEBq)^\dagger$	$2 \cos(kt)$	$-2 \cos(k/2)$	0
$(\pi E0)$	$2(-1)^t$	0	0
$(\pi Em+, \pi Em-)$	$4(-1)^t \cos(m\alpha)$	0	0
$(\pi Eq)^\dagger$	$2(-1)^{t+q}$	0	0

† Only for $q = 2, 4, \dots$

References

- Božović I 1984 *Phys. Rev. B* **29** 6586
 — 1985 *Phys. Rev. B* **32** 8136
 — 1986 *Phys. Rev. B* **33** 5956
 Božović I and Božović N 1989 *J. Phys. A: Math. Gen.* **22** 145
 — 1990 *J. Phys. A: Math. Gen.* **23** 2775
 Božović I and Delhalle J 1984 *Phys. Rev. B* **29** 4733
 Jahn H A and Teller E 1937 *Proc. R. Soc. A* **161** 220
 Kamimura H (ed) 1985 *Theoretical Aspects of Band Structures and Electronic Properties of Pseudo-One-Dimensional Solids* (Dordrecht: Reidel)
 Koch M and Seelig F 1987 *Int. J. Quant. Chem.* **32** 249
 Kuzmany H, Mehring M and Roth S (eds) 1985 *Electronic Properties of Polymers and Related Compounds* (Berlin: Springer)
 Miller J (ed) 1982 *Extended Linear Chain Compounds* (New York: Plenum)
 Monceau P (ed) 1985 *Electronic Properties of Inorganic Quasi-One-Dimensional Compounds* (Dordrecht: Reidel)
 Peierls R E 1955 *Quantum Theory of Solids* (Oxford: Oxford University Press)
 Sherwin M S, Zettl A and Richards P 1986 *Phys. Rev. B* **36** 6708
 Skotheim T 1986 *Handbook of Conducting Polymers* (New York: Dekker)