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Normal vibrations and Jahn-Teller effect for polymers and quasi-one-dimensional systems

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Normal vibrational modes of all possible quasi-one-dimensional systems and polymers are classified according to the line-group symmetry. The results are used to discuss the vibronic instabilities for such systems and to establish the Jahn-Teller theorem. A general, but simple method, involving only one monomer, is developed to construct the normal displacements for the concrete polymers. As an illustration, it is verified that the symmetry arguments confirm the Jahn-Teller effect in *trans*-polyacetylene, resulting in dimerization with alternating bond lengths.

I. INTRODUCTION

Normal vibrational modes are used in many physical calculations. Symmetry considerations yield standard method of their classification. For small molecules the point groups often suffice while for three-dimensional (3D) crystals space groups may be required. A complete classification of the normal modes of molecules is available;[1] many results are known for 3D crystals as well.[2] On the contrary, similar calculations for the systems periodical in one dimension are far from complete, despite the extensive interest for quasi-1D systems and polymers during the past decade. One of the intentions of this paper is to fill in the gap, and to classify the normal modes of such systems. Since a 3D crystal also possesses line-group symmetry as a part of its space group, these results are also applicable in crystal physics.

Jahn and Teller in their classical paper[1] demonstrated that the vibronic coupling would induce configurational instability of the molecule with an electronic orbital degeneracy in the ground state (with the exception of linear molecules). There is no general proof for 3D crystals, although it has been verified for a number of special cases. The solution of this problem for the systems with one-dimensional periodicity (again, only particular examples have been available[3,4]), based on a classification of all possible vibrational modes, is the second objective of the present paper.

Geometrical symmetries of a system periodic in one direction form one of the line groups. There are infinitely many different line groups, gathered into 13 families. Among results on the theory of line groups, their factorizations,[5] irreducible representations,[6] and symmetrized Kronecker squares of real representations[4] will be used here.

To determine the normal vibrational modes of the system S (e.g., molecule, polymer, crystal) of $|S|$ points with the symmetry group G, the usual Wigner's method[7] is applied. Its main part is the reduction of the dynamical representation[2] $S^V(G)$ to the irreducible components. To construct $S^V(G)$, a basis $\{e_x^s, e_y^s, e_z^s\}$ is associated with each point s of S; the action of the group in this space of the displacements gives the matrix $3|S|$-dimensional representation $S^V(G)=S(G)\otimes V(G)$, where $S(G)$ is the permutational $|S|$-dimensional representation of G, manifesting the action[8] of G on S, while $V(G)$ is the polar-vector three-dimensional representation of G. The irreducible components of this representation give normal vibrational, translational, and rotational modes. An important property of the representation $S(G)$ is that it is automatically in the partially reduced form if the system contains several orbits (disjoint union of sets will be denoted as a sum): $S=\sum_{i=1}^{f} S_i$ implies $S(G)=\oplus_{i=1}^{f} S_i(G)$. Then

$$S^V(G)=\oplus_{i=1}^{f} S_i^V(G) , \tag{1}$$

reflecting the independence of $S^V(G)$ on the relative position of the orbits in S. Hence, the problem of the classification of the normal modes includes (i) the classification of the orbits of G and (ii) the reduction of $S_i^V(G)$ to the irreducible components for each orbit S_i. In Secs. II and III these tasks are systematically performed for systems with the line-group symmetry. The outcomes enable one to generalize the classical Jahn-Teller theorem to the line groups (Sec IV). Some applications of the results and calculation of normal displacements are discussed in Sec. V.

II. ORBITS OF THE LINE GROUPS

A derivation of the different types of orbits of the line groups starts with an analysis of the structure of the orbits. In what follows any system periodic in one direction, i.e., a set of points in $\mathbb{R}^3$ having line-group symmetry, will be called a *polymer*, independently of its physical properties. Let S be such a system, with the symmetry group $\mathbf{L}$ (one of the line groups), containing only one orbit. This means that $S=\{s_1,s_2,\dots,\}$ is the denumerable set with the property that for each point s from S the set $\mathbf{L}s=\{ls \mid l\in\mathbf{L}\}$ is equal to S. The subset of the elements of $\mathbf{L}$ for which s is a fixed point is a subgroup of $\mathbf{L}$, called the stabilizer of that point, $\mathbf{L}_s$. It is well known that all the points of S (being a single orbit) have conjugated stabilizers, and therefore orbits with nonconjugated stabilizers are nonequivalent. Also, if $\mathbf{L}=\sum_i l_i\mathbf{L}_s$ (coset decomposition, $l_1=e$, which is the identity of $\mathbf{L}$), then $S=\{l_1s,l_2s,\ldots\}$, implying that the conjugate stabilizers are associated with orbits of the same type,[8] i.e., with the equivalent permutational representation of $\mathbf{L}$. Therefore, the classification of the nonconjugated stabilizers of $\mathbf{L}$ is being sought. For the point groups, this classification is known.[1] This can be combined with specific structural features of the line groups, to produce an easy solution of the present problem.

The most important fact is that each line group is factorizable:[5] $\mathbf{L}=\mathbf{Z}\mathbf{P}$, where $\mathbf{Z}$ is an infinitely denumerable cyclic group acting freely on $\mathbb{R}^3$ (only the identity of $\mathbf{Z}$ is contained in the stabilizers), while $\mathbf{P}$ is an axial point group (a point group whose elements leave the z axis invariant). Both are subgroups of $\mathbf{L}$ having only the identity in common. There are two types of the axial point groups: those without elements reversing the z axis, $\mathbf{P}^+$, and those containing such elements, $\mathbf{P}^-$. In the latter case there is an index-2 subgroup of the $\mathbf{P}^+$ type while all the transformations reversing the z axis form the coset: $\mathbf{P}^-=\mathbf{P}^++B\mathbf{P}^+$. The generator of $\mathbf{Z}$ is the Seitz operator $\mathbf{z}=(Z|\xi)$, translating points for $\xi\neq 0$ along the z axis after the orthogonal transformation Z, which leaves the direction of z (the identity, a rotation around z or the reflection in a vertical plane).

Since $\mathbf{L}_s$ is a subgroup of the factorizable group $\mathbf{L}$, and $\mathbf{L}_s\cap\mathbf{Z}=\{e\}$, its most general form is given by the coset decomposition with respect to the subgroup $\mathbf{P}_s=\mathbf{P}\cap\mathbf{L}_s$: $\mathbf{L}_s=\sum_i\mathbf{z}^ip_i\mathbf{P}_s$, where $\mathbf{z}^i$ and p_i are from $\mathbf{Z}$ and $\mathbf{P}$, respectively ($\mathbf{z}^0=p_0=e$). Two cases can be distinguished:[9] (a) $\mathbf{L}_s=\mathbf{P}_s$ and (b) there are cosets of $\mathbf{P}_s$ in $\mathbf{L}_s$.

In the latter case, p_i must reverse the z axis, since otherwise $\mathbf{z}^ip_i$ has no fixed points for $\mathbf{z}^i\neq e$, and cannot be in the stabilizer: $\mathbf{L}_s=\sum_i\mathbf{z}^iBp_i{}^+\mathbf{P}_s$, where $p_i{}^+$ are from $\mathbf{P}^+$, and $\mathbf{P}_s$ is a subgroup of $\mathbf{P}^+$, precisely $\mathbf{P}_s=\mathbf{P}_s^+=\mathbf{L}_s\cap\mathbf{P}^+$. For any two coset representatives $\mathbf{z}^iBp_i{}^+$ and $\mathbf{z}^jBp_j{}^+(i,j\neq 1)$, the product $(\mathbf{z}^iBp_i{}^+)^{-1}\mathbf{z}^jBp_j{}^+$ must be in $\mathbf{L}_s$, while a simple calculation gives that this composite transformation diminishes the z coordinate of s for $\xi_j-\xi_i$, implying $\mathbf{z}^i=\mathbf{z}^j$. But in this case also $p_i{}^+=p_j{}^+$. Therefore, there is at most one coset: $\mathbf{L}_s=\mathbf{P}_s^++\mathbf{z}^kBp^+\mathbf{P}_s^+$. Conjugation by $\mathbf{z}^t$ easily verifies that $\mathbf{L}_s$ is conjugated to a subgroup of type (a) for k even, and otherwise to a subgroup of type (b) but with $k=1$.

To summarize, there are two types of stabilizers:

$$\mathbf{L}_s=\mathbf{P}_s\ , \tag{2a}$$

$$\mathbf{L}_s=\mathbf{P}_s^++\mathbf{z}A\mathbf{P}_s^+\ , \tag{2b}$$

with $A=Bp^+$. Stabilizers of type (2a) are the stabilizers of the axial point group $\mathbf{P}$, which are known, while the second case can arise only for the 9 families of the line groups with the elements reversing the z axis. Even in this case, all the subgroups $\mathbf{P}_s^+$ are the stabilizers of the point group $\mathbf{P}^+$, and what remains to be done is to calculate possible combinations $\mathbf{z}A$. Since $\mathbf{L}_s$ is a subgroup, the conditions (i) $(\mathbf{z}A)^2\in\mathbf{P}_s^+$ (reduces to $A^2\in\mathbf{P}_s^+$ if $\mathbf{Z}$ is an invariant subgroup) and (ii) $A\mathbf{P}_s^+=\mathbf{P}_s^+A$ (or, equivalently, A belongs to the normalizer of $\mathbf{P}_s^+$ in $\mathbf{P}$) must be fulfilled.

The classifying algorithm for the $\mathbf{L}$-orbits becomes quite straightforward at this instant. If $\mathbf{P}=\mathbf{P}^+$, each orbit type of $\mathbf{P}$ generates exactly one orbit type of $\mathbf{L}$, giving the complete set of $\mathbf{L}$-orbits. It turns out that this correspondence is bijective, except in the case of the group $\mathbf{L}(2n)_nmc$ (n even), when the point group orbits b and c generate the same orbit type of the line group (stabilizers are conjugated by the generator of $\mathbf{Z}$). In the case $\mathbf{P}=\mathbf{P}^-$, orbit types of $\mathbf{P}$ with the stabilizers reversing the z axis bijectively correspond to a part of $\mathbf{L}$-orbit types. However, $\mathbf{P}$-orbit type with the stabilizer from $\mathbf{P}^+$ (only orthogonal transformations are considered) is in general split when $\mathbf{Z}$ is introduced: (a) there are points in $\mathbb{R}^3$ for which $\mathbf{P}_s^+$ remains the stabilizer in $\mathbf{L}$, and they give one $\mathbf{L}$-orbit type (again, the correspondence is bijective, except that for the groups $\mathbf{L}(2n)_n/mcm$, where point group orbits b and c generate the same orbit type of the line group); (b) for other points stabilizer in $\mathbf{Z}$ is doubled. In this case all the subgroups of the type (2b) would be found [using conditions (i) and (ii) above], and among them only those for which $\mathbf{P}_s^+$ and the coset had the same fixed points would be retained. Finally, nonconjugated subgroups obtained in this manner generate bijectively the rest of the $\mathbf{L}$-orbit types. The results of this procedure (being much more simple to apply than to explain) are given in Table I. In this table the following factorizations of the line groups are used:

1. $\mathbf{q}_r\mathbf{C}_n=\mathbf{L}q_{\underline{p}}\ \underline{,}$
2. $\mathbf{TS}_{2n}=\mathbf{L}(2n),\mathbf{L}\bar{n}\ \underline{,}$
3. $\mathbf{TC}_{nh}=\mathbf{L}n/m,\mathbf{L}(\overline{2n})\ ,$
4. $(2\mathbf{n})_1\mathbf{C}_{nh}=\mathbf{L}(2n)_n/m\ ,$
5. $\mathbf{q}_r\mathbf{D}_n=\mathbf{L}q_p22,\mathbf{L}q_p2\ ,$
6. $\mathbf{TC}_{nv}=\mathbf{L}nmm,\mathbf{L}nm\ ,$
7. $\mathbf{T}_c\mathbf{C}_n=\mathbf{L}ncc,\mathbf{L}nc\ ,$
8. $(2\mathbf{n})_1\mathbf{C}_{nv}=\underline{\mathbf{L}}(2n)_nmc\ ,$
9. $\mathbf{TD}_{nd}=\mathbf{L}(2\underline{n\,)}2m,\mathbf{L}\bar{n}m\ ,$
10. $\mathbf{T}_c\mathbf{S}_{2n}=\mathbf{L}(\overline{2n})2c,\mathbf{L}\bar{n}c\ \underline{,}$
11. $\mathbf{TD}_{nh}=\mathbf{L}n/mmm,\mathbf{L}(\underline{2}n)2m\ ,$
12. $\mathbf{T}_c\mathbf{C}_{nh}=\mathbf{L}n/mcc,\mathbf{L}(\overline{2n})2c\ ,$
13. $(2\mathbf{n})_1\mathbf{D}_{nh}=\mathbf{L}(2n)_n/mcm\ .$

For families 1 and 5, the cases when $\mathbf{q}_r$ is $\mathbf{T}$ and $(2\mathbf{n})_1$ are separately considered in the table for the purposes of the next section.

After this discussion on the stabilizers, a brief consideration of the corresponding orbits will be made. The whole polymer must be disjoint union of the orbits of $\mathbf{Z}$. Each $\mathbf{Z}$ orbit has $|\mathbf{Z}|$ points, since the action of $\mathbf{Z}$ is free. This enables us to form the *monomer* Y, the set containing a point from each of these orbits. Then the polymer S is generated from Y by the action of $\mathbf{Z}$ in the form of disjoint union: $S=\sum_{t=-\infty}^{\infty}\mathbf{z}^tY$, with $|S|=|Y|\,|\mathbf{Z}|$.

If S is an $\mathbf{L}$-orbit of type (2a) there is no p in $\mathbf{P}$ and $\mathbf{z}^i$ in $\mathbf{Z}$ such that $ps=\mathbf{z}^is$, otherwise $\mathbf{z}^{-i}p$ belongs to $\mathbf{L}_s$. In other words S is factorized into orbits of $\mathbf{P}$ and orbits of $\mathbf{Z}$, giving the simple form of the monomer:

TABLE I. Orbit types of the line groups. For each line group $\mathbf{L}=\mathbf{ZP}$ its orbit types are given in the intersection of row $\mathbf{P}$ and column $\mathbf{Z}$. At some places $\mathbf{Z}$ and $\mathbf{P}$ do not combine into a group, or the resulting group is treated within another factorization. For the orbits with the stabilizer $\mathbf{P}_s+\mathbf{z}A\mathbf{P}_s$, $\mathbf{P}_s$ is presented in the fourth column and A under the corresponding $\mathbf{Z}$ factor (hence, if the stabilizer is $\mathbf{P}_s$ only, "None" is under $\mathbf{Z}$). For $\mathbf{Z}$ equal to $\mathbf{T}$, $(\mathbf{2n})_1$, $\mathbf{q}_r$, and $\mathbf{T}_c$, the generators $\mathbf{z}$ are $(E|0)$, $(C_{2n}|\frac{1}{2})$, $(C_q^r|n/q)$, and $(\sigma_v|\frac{1}{2})$, respectively (the unit of the translational part is the translational period). Symbols $a,b,\ldots,$ for orbits are as in Ref. 1, with indices to distinguish different $\mathbf{L}$-orbit types generated from the same $\mathbf{P}$-orbit type. The number in the third column is the order of the monomer. Note that σ_h is the reflection in xy plane, while σ_v and U are along the x axis, except in $\mathbf{D}_{nd}$ where only σ_v is along the x axis. In the fifth column the maximal axial point group leaving the monomer invariant is given.

$\mathbf{P}$	Orbit	$\lvert Y\rvert$	$\mathbf{P}_s$	Axial group	$\mathbf{T}$	$(\mathbf{2n})_1$	$\mathbf{q}_r$	$\mathbf{T}_c$
$\mathbf{C}_n$	a	n	$\mathbf{C}_1$	$\mathbf{D}_{nh}$	None	None	None	None
	b_1	1	$\mathbf{C}_n$	$\mathbf{D}_{\infty h}$	None	None	None	None
$\mathbf{S}_{2n}$	a_1	$2n$	$\mathbf{C}_1$	$\mathbf{D}_n$	None	$(\mathbf{2n})_1\mathbf{C}_{nh}$	Not group	None
n odd	a_2	n			\			$C_{2n}^n\sigma_h$
	b_1	2	$\mathbf{C}_n$	$\mathbf{D}_{\infty h}$	None			None
	b_2	1			$C_{2n}\sigma_h$			$C_{2n}\sigma_h$
	c_1	1	$\mathbf{S}_{2n}$	$\mathbf{D}_{\infty h}$	None			None
$\mathbf{C}_{nh}$	a_1	$2n$	$\mathbf{C}_1$	$\mathbf{D}_{nh}$	None	None	Not group	None
	a_2	n			σ_h	\		σ_h
$n=4k+2$	a_3	n			\	\		σ_hC_n
	b_1	n	$\mathbf{C}_{1h}$	$\mathbf{D}_{nh}$	None	None		None
	c_1	2	$\mathbf{C}_n$	$\mathbf{D}_{\infty h}$	None	None		None
	c_2	1		$\mathbf{D}_{\infty h}$	σ_h	σ_h		σ_h
	d_1	1	$\mathbf{C}_{nh}$	$\mathbf{D}_{\infty h}$	None	None		None
$\mathbf{C}_{nv}$	a_1	$2n$	$\mathbf{C}_1$	$\mathbf{D}_{nh}$	None	None	Not group	$(\mathbf{2n})_1\mathbf{C}_{nv}$
	b_1	n	$\mathbf{C}_{1v}$	$\mathbf{D}_{nh}$	None	None		$\mathbf{TC}_{nv}$
n even	c_1	n	$\mathbf{C}_{1v}$	$\mathbf{D}_{nh}$	None	\		
	d_1	1	$\mathbf{C}_{nv}$	$\mathbf{D}_{\infty h}$	None	None		
$\mathbf{D}_n$	a_1	$2n$	$\mathbf{C}_1$	$\mathbf{D}_n$	None	None	None	$\mathbf{T}_c\mathbf{S}_{2n}$
	a_2	n			U	U	U	$\mathbf{T}_c\mathbf{C}_{nh}$
n even	a_3	n			UC_n	UC_n	UC_n	
	b_1	n	$\mathbf{D}_1$	$\mathbf{D}_{nh}$	None	None	None	
n even	c_1	n	$\mathbf{D}_1$	$\mathbf{D}_{nh}$	None	None	None	
	d_1	2	$\mathbf{C}_n$	$\mathbf{D}_{\infty h}$	None	None	None	
	d_2	1			U	U	U	
	e_1	1	$\mathbf{D}_n$	$\mathbf{D}_{\infty h}$	None	None	None	
$\mathbf{D}_{nd}$	a_1	$4n$	$\mathbf{C}_1$	$\mathbf{D}_{nd}$	None	$(\mathbf{2n})_1\mathbf{D}_{nh}$	Not group	$\mathbf{TD}_{nd}$
	a_2	$2n$			U			
	b_1	$2n$	$\mathbf{C}_{1v}$	$\mathbf{D}_{nd}$	None			
	c_1	$2n$	$\mathbf{D}_1$	$\mathbf{D}_{2nh}$	None			
	d_1	2	$\mathbf{C}_{nv}$	$\mathbf{D}_{\infty h}$	None			
	d_2	1			U			
	e_1	1	$\mathbf{D}_{nd}$	$\mathbf{D}_{\infty h}$	None			
$\mathbf{D}_{nh}$	a_1	$4n$	$\mathbf{C}_1$	$\mathbf{D}_{nh}$	None	None	Not group	$\mathbf{TD}_{nh}$
	a_2	$2n$			σ_h	U		$(\mathbf{2n})_1\mathbf{D}_{nh}$
	b_1	$2n$	$\mathbf{C}_{1v}$	$\mathbf{D}_{nh}$	None	None		$\mathbf{T}_c\mathbf{D}_{nd}$
	b_2	n			σ_h	\		
n even	c_1	$2n$	$\mathbf{C}_{1v}$	$\mathbf{D}_{nh}$	None	\		
n even	c_2	n			σ_h	\		
	d_1	$2n$	$\mathbf{C}_{1h}$	$\mathbf{D}_{nh}$	None	None		
	e_1	n	$\mathbf{D}_{1h}$	$\mathbf{D}_{nh}$	None	None		
n even	f_1	n	$\mathbf{D}_{1h}$	$\mathbf{D}_{nh}$	None	None		
	g_1	2	$\mathbf{C}_{nv}$	$\mathbf{D}_{\infty h}$	None	None		
	g_2	1			σ_h	σ_h		
	h_1	1	$\mathbf{D}_{nh}$	$\mathbf{D}_{\infty h}$	None	None		

$Y=\mathbf{P}s=\{ps \mid p\in\mathbf{P}\}$, i.e., one monomer is the orbit of $\mathbf{P}$ with s, and $|S|=|\mathbf{Z}|\,|\mathbf{P}|/|\mathbf{P}_s|$. In the case when S is of type (2b), $\mathbf{z}^{-1}s=As$, and clearly $\mathbf{P}s=\mathbf{P}^{+}s+\mathbf{z}\mathbf{P}^{+}s$ (to show this in detail, note that $\mathbf{z}\mathbf{P}^{+}=\mathbf{P}^{+}\mathbf{z}$ and $A\mathbf{P}^{+}=\mathbf{P}^{+}A$). Hence, the role of monomer is taken by $Y=\mathbf{P}^{+}s$, and the order of the orbit is $|S|=|\mathbf{Z}|\,|\mathbf{P}|/2|\mathbf{P}_s|$.

III. DYNAMICAL REPRESENTATIONS

The character $\sigma(l)$ of the element $l=\mathbf{z}^t p$ in the representation $S(\mathbf{L})$ is exactly the number of the fixed points of l in S, and can be found by use of the induction method.[10] In fact, the action of $\mathbf{L}$ on S is induced from the action on the monomers. In cases (2a) and (2b) the maximal subgroups of $\mathbf{L}$ leaving Y invariant are $\mathbf{P}$ and $\mathbf{P}^{z}=\mathbf{P}^{+}+\mathbf{z}A\mathbf{P}^{+}$, respectively ($Y$ is the orbit of these subgroups). If $Y(\mathbf{P})$ and $Y(\mathbf{P}^{z})$ is their action on the corresponding monomers (with character y), then the action of $\mathbf{L}$ on S is the induced representation: $S(\mathbf{L})=Y(\mathbf{P})\uparrow\mathbf{L}$, for case (2a), and $S(\mathbf{L})=Y(\mathbf{P}^{z})\uparrow\mathbf{L}$, case (2b). In the both cases $\mathbf{Z}$ is a transversal of $\mathbf{L}$ with respect to monomer. Then a straightforward calculation gives (p is an element from $\mathbf{P}^{+}$)

$$\sigma(\mathbf{z}^t p)=\delta_{t,0}\sum_{k=-\infty}^{\infty} y(\mathbf{z}^{-k} p\,\mathbf{z}^{k}) , \tag{3}$$

and, for the elements reversing the z axis in cases (2a) and (2b):

$$\sigma(\mathbf{z}^t Ap)=\begin{cases}0\ , & t\ \text{odd}\ ,\\ y(\mathbf{z}^{t/2}Ap\,\mathbf{z}^{t/2})\ , & t\ \text{even}\ ,\end{cases} \tag{3a}$$

$$\sigma(\mathbf{z}^t Ap)=\begin{cases}y(\mathbf{z}^{(t+1)/2}Ap\,\mathbf{z}^{(t-1)/2}), & t\ \text{odd}\ ,\\ 0\ , & t\ \text{even}\ .\end{cases} \tag{3b}$$

Combining these considerations with the results from Table I the characters of the representations $S(\mathbf{L})$ for each orbit S can be calculated. After that, the characters for the representations $S^{V}(\mathbf{L})$ are easily found using the known characters of the polar-vector representations of the line groups.[11] Indeed, if $v(l)$ denotes the character of $V(l)$ [which is real as well as $S^{V}(\mathbf{L})$], the μth irreducible representation of $\mathbf{L}$, ($\chi^{(\mu)}$ is its character) occurs in the decomposition of $S^{V}(\mathbf{L})$ exactly[10]

$$a_\mu=\frac{1}{|\mathbf{L}|}\sum_{t=-\infty}^{\infty}\sum_{p\in P}\chi^{(\mu)}(\mathbf{z}^t p)\sigma(\mathbf{z}^t p)v(\mathbf{z}^t p)$$

times. Using (3), the last equation reduces to the decomposition on the monomer

$$a_\mu=\frac{1}{|\mathbf{P}|}\sum_{l}\chi^{(\mu)}(l)y(l)v(l) , \tag{4}$$

where the summation is performed over the symmetry group of the monomer, i.e., l is from $\mathbf{P}$ and $\mathbf{P}^{z}$ in cases (2a) and (2b), respectively. This equation provides a simple way to decompose the representations S^{V} for all the orbits of the line groups. The results are presented in Tables II–XIV. Note that the irreducible representations of the line groups $\mathbf{L}q_p$ and $\mathbf{L}q_p2$, $\mathbf{L}q_p22$ (Tables II and VI) differ from the standard ones;[6] a more appropriate form for these purposes is derived in the Appendix.

TABLE II. Vibrational representations of the orbits of the line groups $\mathbf{L}q_p$ $q=1,2,\ldots$; $p=0,\ldots,q-1$. n is the greatest common divisor of q and p. Translational period is q/n units. Summation is performed over $k\in(-\pi,\pi]$, $m\in(-n/2,n/2]$. Minimal sets: $2a$.

Orbit	Orbit point	Vibrational representation
a_1	(x,y,z)	$3\sum_{k,m} {}_{k}A_m$
b_1	$(0,0,0)$	$\sum_{k}({}_{k}A_o+{}_{k}A_1+{}_{k}A_{-1})$

TABLE III. Vibrational representations of the orbits of the line groups $\mathbf{L}(\overline{2n})$ and $\mathbf{L}\bar{n}$; $n=1,2,\ldots$; translational period is 1 unit. Summation is performed over $k\in(0,\pi)$, $m\in(-n/2,n/2]$. Minimal sets: $2a$.

Orbit	Orbit point	Vibrational representation
a_1	(x,y,z)	$3\sum_{m}({}_{o}A_m^{-}+{}_{o}A_m^{+}+{}_{\pi}A_m^{-}+{}_{\pi}A_m^{+})+6\sum_{k,m}{}_{k}^{-k}E_m$
b_1	$(0,0,z)$	$3({}_{o}A_o^{-}+{}_{o}A_o^{+}+{}_{\pi}A_o^{-}+{}_{\pi}A_o^{+})+6\sum_{k}{}_{k}^{-k}E_o;\ n=1$ ${}_{o}A_o^{-}+{}_{o}A_o^{+}+{}_{\pi}A_o^{-}+{}_{\pi}A_o^{+}+2({}_{o}A_1^{-}+{}_{o}A_1^{+}+{}_{\pi}A_1^{-}+{}_{\pi}A_1^{+})+\sum_{k}(2{}_{k}^{-k}E_o+4{}_{k}^{-k}E_1);\ n=2$ ${}_{o}A_o^{-}+{}_{o}A_o^{+}+{}_{\pi}A_o^{-}+{}_{\pi}A_o^{+}+{}_{o}A_1^{-}+{}_{o}A_1^{+}+{}_{o}A_{-1}^{-}+{}_{o}A_{-1}^{+}+{}_{\pi}A_1^{-}+{}_{\pi}A_1^{+}+{}_{\pi}A_{-1}^{-}+{}_{\pi}A_{-1}^{+}+$ $+2\sum_{k}({}_{k}^{-k}E_o+{}_{k}^{-k}E_1+{}_{k}^{-k}E_{-1});\ n>2$
b_2	$(0,0,\frac{1}{2})$	$3({}_{o}A_o^{-}+{}_{\pi}A_o^{+})+3\sum_{k}{}_{k}^{-k}E_o;\ n=1$ ${}_{o}A_o^{-}+{}_{\pi}A_o^{+}+{}_{o}A_1^{+}+{}_{\pi}A_1^{-}+{}_{o}A_1^{-}+{}_{\pi}A_1^{+}+\sum_{k}({}_{k}^{-k}E_o+2{}_{k}^{-k}E_1);\ n=2$ ${}_{o}A_o^{-}+{}_{\pi}A_o^{+}+{}_{o}A_1^{+}+{}_{o}A_{-1}^{+}+{}_{\pi}A_1^{-}+{}_{\pi}A_{-1}^{-}+\sum_{k}({}_{k}^{-k}E_o+{}_{k}^{-k}E_1+{}_{k}^{-k}E_{-1});\ n>2$
c_1	$(0,0,0)$	$3({}_{o}A_o^{-}+{}_{\pi}A_o^{-})+3\sum_{k}{}_{k}^{-k}E_o;\ n=1$ ${}_{o}A_o^{-}+{}_{\pi}A_o^{-}+{}_{o}A_1^{+}+{}_{\pi}A_1^{+}+{}_{o}A_1^{-}+{}_{\pi}A_1^{-}+\sum_{k}({}_{k}^{-k}E_o+2{}_{k}^{-k}E_1);\ n=2$ ${}_{o}A_o^{-}+{}_{\pi}A_o^{-}+{}_{o}A_1^{+}+{}_{o}A_{-1}^{+}+{}_{\pi}A_1^{+}+{}_{\pi}A_{-1}^{+}+\sum_{k}({}_{k}^{-k}E_o+{}_{k}^{-k}E_1+{}_{k}^{-k}E_{-1});\ n>2$

TABLE IV. Vibrational representations of the orbits of the line groups $\mathbf{L}n/m$ and $\mathbf{L}(\overline{2n})$ $n=1,2,\ldots$; translational period is 1 unit. Summation is performed over $k\in(0,\pi)$, $m\in(-n/2,n/2]$. Minimal sets: $2a$, $2b$, or $a+b$.

Orbit	Orbit point	Vibrational representation
a_1	(x,y,z)	$3\sum_m({}_0A_m^- + {}_0A_m^+ + {}_\pi A_m^- + {}_\pi A_m^+) + 6\sum_{k,m}{}_k^{-k}E_m$
a_2	$(x,y,\frac{1}{2})$	$\sum_m[{}_0A_m^- + {}_\pi A_m^+ + 2({}_0A_m^+ + {}_\pi A_m^-)] + 3\sum_{k,m}{}_k^{-k}E_m$
b_1	$(x,y,0)$	$\sum_m[{}_0A_m^- + {}_\pi A_m^- + 2({}_0A_m^+ + {}_\pi A_m^+)] + 3\sum_{k,m}{}_k^{-k}E_m$
c_1	$(0,0,z)$	$3({}_0A_0^- + {}_0A_0^+ + {}_\pi A_0^- + {}_\pi A_0^+) + 6\sum_k{}_k^{-k}E_0;\ n=1$ ${}_0A_0^- + {}_0A_0^+ + {}_\pi A_0^- + {}_\pi A_0^+ + 2({}_0A_1^- + {}_0A_1^+ + {}_\pi A_1^- + {}_\pi A_1^+) + 2\sum_k({}_k^{-k}E_0 + 2{}_k^{-k}E_1);\ n=2$ ${}_0A_0^- + {}_0A_0^+ + {}_\pi A_0^- + {}_\pi A_0^+ + {}_0A_1^- + {}_0A_1^+ + {}_0A_{-1}^- + {}_0A_{-1}^+ + {}_\pi A_1^- + {}_\pi A_1^+ + {}_\pi A_{-1}^- + {}_\pi A_{-1}^+ +$ $+2\sum_k({}_k^{-k}E_0 + {}_k^{-k}E_1 + {}_k^{-k}E_{-1});\ n>2$
c_2	$(0,0,\frac{1}{2})$	$2({}_0A_0^+ + {}_\pi A_0^-) + {}_0A_0^- + {}_\pi A_0^+ + 3\sum_k{}_k^{-k}E_0;\ n=1$ ${}_0A_0^- + {}_\pi A_0^+ + 2({}_0A_1^+ + {}_\pi A_1^-) + \sum_k({}_k^{-k}E_0 + 2{}_k^{-k}E_1);\ n=2$ ${}_0A_0^- + {}_\pi A_0^+ + {}_0A_1^+ + {}_0A_{-1}^+ + {}_\pi A_1^- + {}_\pi A_{-1}^- + \sum_k({}_k^{-k}E_0 + {}_k^{-k}E_1 + {}_k^{-k}E_{-1});\ n>2$
d_1	$(0,0,0)$	$2({}_0A_0^+ + {}_\pi A_0^+) + {}_0A_0^- + {}_\pi A_0^- + 3\sum_k{}_k^{-k}E_0;\ n=1$ ${}_0A_0^- + {}_\pi A_0^- + 2({}_0A_1^+ + {}_\pi A_1^+) + \sum_k({}_k^{-k}E_0 + 2{}_k^{-k}E_1);\ n=2$ ${}_0A_0^- + {}_\pi A_0^- + {}_0A_1^+ + {}_0A_{-1}^+ + {}_\pi A_1^+ + {}_\pi A_{-1}^+ + \sum_k({}_k^{-k}E_0 + {}_k^{-k}E_1 + {}_k^{-k}E_{-1});\ n>2$

IV. JAHN-TELLER THEOREM FOR POLYMERS

The Jahn-Teller theorem asserts that for any degenerate electronic state, some normal modes of the phonon spectrum will be activated due to the vibronic coupling, to produce nonsymmetrical distortion of the ions. The exceptions are the linear ion configurations as well as the electronic Kramers's degeneracy.

From the group theoretical point of view, electronic orbital degeneracy means that the state $|E\rangle$ of the polymer's electronic subsystem belongs to the multidimensional real irreducible representation $E(\mathbf{L})$. In the linear vibronic coupling, the mean value, $\langle E|H|E\rangle$, of the Hermitian real operator, transforming according to the irreducible component $D^H(\mathbf{L})$ of the representation $S^V(\mathbf{L})$ (S is the ion configuration), multiplies the normal mode Q^H associated to this representation. Hence, when $\langle E|H|E\rangle\neq 0$ this mode is active. If it is not the totally symmetric, translational, or rotational mode, the polymer S will be distorted. The Jahn-Teller theorem points out that such active modes always exist, i.e., that for each $E(\mathbf{L})$, its symmetrized square $[E^2(\mathbf{L})]$ contains common irreducible components with $S^V(\mathbf{L})$ (here symmetrical, translational, and rotational representations are not

TABLE V. Vibrational representations of the orbits of the line groups $\mathbf{L}(2n)_n/m$. Summation is performed over $k\in(0,\pi)$. Translational period is 1 unit. In the primed sums m is from $(0,n]$, otherwise from $(-n,n]$. Minimal sets: $2a$, $2b$, or $a+b$.

Orbit	Orbit point	Vibrational representation
a_1	(x,y,z)	$3\sum_m({}_0A_m^+ + {}_0A_m^-) + 6\sum_{k,m}{}_k^{-k}E_m + 6\sum_m{}'\,{}_\pi E_m^{m-n}$
b_1	$(x,y,0)$	$\sum_m({}_0A_m^- + 2{}_0A_m^+) + 3\sum_{k,m}{}_k^{-k}E_m + 3\sum_m{}'\,{}_\pi E_m^{m-n}$
c_1	$(0,0,z)$	$3({}_0A_0^- + {}_0A_0^+ + {}_0A_1^- + {}_0A_1^+) + 6\sum_k({}_k^{-k}E_0 + {}_k^{-k}E_1) + 6{}_\pi E_1^0;\ n=1$ ${}_0A_0^- + {}_0A_0^+ + {}_0A_1^- + {}_0A_1^+ + {}_0A_{-1}^- + {}_0A_{-1}^+ + {}_0A_{n-1}^- + {}_0A_{n-1}^+ + {}_0A_{-n+1}^- + {}_0A_{-n+1}^+ + {}_0A_n^+ + {}_0A_n^- +$ $+2({}_\pi E_{n-1}^{-1} + {}_\pi E_1^{1-n} + {}_\pi E_n^0) + 2\sum_k({}_k^{-k}E_0 + {}_k^{-k}E_1 + {}_k^{-k}E_{-1} + {}_k^{-k}E_n + {}_k^{-k}E_{n-1} + {}_k^{-k}E_{-n+1});\ n>1$
c_2	$(0,0,\frac{1}{4})$	$3({}_0A_1^+ + {}_0A_0^-) + 3\sum_k({}_k^{-k}E_0 + {}_k^{-k}E_1) + 3{}_\pi E_1^0;\ n=1$ ${}_0A_0^- + {}_0A_1^+ + {}_0A_{-1}^+ + {}_0A_n^+ + {}_0A_{n-1}^- + {}_0A_{-n+1}^- + {}_\pi E_{n-1}^{-1} + {}_\pi E_1^{1-n} + {}_\pi E_n^0 +$ $+\sum_k({}_k^{-k}E_0 + {}_k^{-k}E_1 + {}_k^{-k}E_{-1} + {}_k^{-k}E_n + {}_k^{-k}E_{n-1} + {}_k^{-k}E_{-n+1});\ n>1$
d_1	$(0,0,0)$	$2({}_0A_0^+ + {}_0A_1^+) + {}_0A_0^- + {}_0A_1^- + 3\sum_k({}_k^{-k}E_0 + {}_k^{-k}E_1) + {}_\pi E_1^0;\ n=1$ ${}_0A_0^- + {}_0A_1^+ + {}_0A_{-1}^+ + {}_0A_n^- + {}_0A_{n-1}^+ + {}_0A_{-n+1}^+ + {}_\pi E_{n-1}^{-1} + {}_\pi E_1^{1-n} + {}_\pi E_n^0 +$ $+\sum_k({}_k^{-k}E_0 + {}_k^{-k}E_1 + {}_k^{-k}E_{-1} + {}_k^{-k}E_n + {}_k^{-k}E_{n-1} + {}_k^{-k}E_{-n+1});\ n>1$

TABLE VI. Vibrational representations of the orbits of the line groups **L**q_p22 and **L**q_p2; $q=1,2,\ldots$; $p=0,\ldots,q-1$. Translational period is q/n units. n is the greatest common divisor of q and p. Summation is performed over $k\in(0,\pi)$. In the primed sums m is from $(0,n/2)$, otherwise from $(-n/2,n/2)$. $c=\rho\cos(\pi/n)$ and $s=\rho\sin(\pi/n)$. Orbits c_1 and a_3 exist for n even, only. Minimal sets: a for **L**$n2$, **L**$n22$ and **L**$(2n)_n22$, and a, b, c otherwise.

Orbit	Orbit point	Vibrational representation
a_1 n even	(x,y,z)	$3({}_oA_o^+ + {}_oA_o^- + {}_\pi A_o^+ + {}_\pi A_o^-) + 6{\sum_m}'({}_\pi E_m + {}_oE_m) + 6\sum_{k,m}{}_k^{-k}E_m^{-m}+$ $+3({}_oA_{n/2}^+ + {}_oA_{n/2}^- + {}_\pi A_{n/2}^+ + {}_\pi A_{n/2}^-) + 6\sum_k {}_kE_{n/2}$
a_2 n even	$(x,0,\frac{1}{2})$	${}_oA_o^+ + {}_\pi A_o^- + 2({}_oA_o^- + {}_\pi A_o^+) + 3{\sum_m}'({}_\pi E_m + {}_oE_m) + 3\sum_{k,m}{}_k^{-k}E_m^{-m}+$ $+{}_oA_{n/2}^+ + {}_\pi A_{n/2}^- + 2({}_oA_{n/2}^- + {}_\pi A_{n/2}^+) + 3\sum_k {}_kE_{n/2}$
a_3	$(c,s,\frac{1}{2})$	${}_oA_o^+ + {}_oA_{n/2}^- + {}_\pi A_o^- + {}_\pi A_{n/2}^+ + 2({}_oA_o^- + {}_oA_{n/2}^+ + {}_\pi A_o^+ + {}_\pi A_{n/2}^-) + 3\sum_k {}_kE_{n/2}+$ $+3{\sum_m}'({}_\pi E_m + {}_oE_m) + 3\sum_{k,m}{}_k^{-k}E_m^{-m}$
b_1 n even	$(x,0,0)$	${}_oA_o^+ + {}_\pi A_o^+ + 2({}_oA_o^- + {}_\pi A_o^-) + 3{\sum_m}'({}_\pi E_m + {}_oE_m) + 3\sum_{k,m}{}_k^{-k}E_m^{-m}+$ $+{}_oA_{n/2}^+ + {}_\pi A_{n/2}^+ + 2({}_oA_{n/2}^- + {}_\pi A_{n/2}^-) + 3\sum_k {}_kE_{n/2}$
c_1	$(c,s,0)$	${}_oA_o^+ + {}_oA_{n/2}^- + {}_\pi A_o^+ + {}_\pi A_{n/2}^- + 2({}_oA_o^- + {}_oA_{n/2}^+ + {}_\pi A_o^- + {}_\pi A_{n/2}^+) + 3\sum_k {}_kE_{n/2}+$ $+3{\sum_m}'({}_\pi E_m + {}_oE_m) + 3\sum_{k,m}{}_k^{-k}E_m^{-m}$
d_1	$(0,0,z)$	$6\sum_k {}_k^{-k}E_o + 3({}_oA_o^+ + {}_oA_o^- + {}_\pi A_o^+ + {}_\pi A_o^-)$; $n=1$ $\sum_k(2{}_k^{-k}E_o + 4{}_k^{-k}E_1) + {}_oA_o^+ + {}_oA_o^- + {}_\pi A_o^+ + {}_\pi A_o^- + 2({}_oA_1^+ + {}_oA_1^- + {}_\pi A_1^+ + {}_\pi A_1^-)$; $n=2$ $2\sum_k({}_k^{-k}E_o + {}_k^{-k}E_1 + {}_k^{-k}E_{-1}) + {}_oA_o^+ + {}_oA_o^- + {}_\pi A_o^+ + {}_\pi A_o^- + 2({}_\pi E_1 + {}_oE_1)$; $n>2$
d_2	$(0,0,\frac{1}{2})$	$3\sum_k {}_k^{-k}E_o + {}_oA_o^+ + {}_\pi A_o^- + 2({}_oA_o^- + {}_\pi A_o^+)$; $n=1$ $\sum_k({}_k^{-k}E_o + 2{}_k^{-k}E_1) + {}_oA_o^- + {}_\pi A_o^+ + {}_oA_1^+ + {}_oA_1^- + {}_\pi A_1^+ + {}_\pi A_1^-$; $n=2$ $\sum_k({}_k^{-k}E_o + {}_k^{-k}E_1 + {}_k^{-k}E_{-1}) + {}_oA_o^- + {}_\pi A_o^+ + {}_\pi E_1 + {}_oE_1$; $n>2$
e_1	$(0,0,0)$	$3\sum_k {}_k^{-k}E_o + {}_oA_o^+ + {}_\pi A_o^+ + 2({}_oA_o^- + {}_\pi A_o^-)$; $n=1$ $\sum_k({}_k^{-k}E_o + 2{}_k^{-k}E_1) + {}_oA_o^- + {}_\pi A_o^- + {}_oA_1^+ + {}_oA_1^- + {}_\pi A_1^+ + {}_\pi A_1^-$; $n=2$ $\sum_k({}_k^{-k}E_o + {}_k^{-k}E_1 + {}_k^{-k}E_{-1}) + {}_oA_o^- + {}_\pi A_o^- + {}_\pi E_1 + {}_oE_1$; $n>2$

counted).

In general, the polymer S with the group of symmetry **L** is a union of orbits $S=S_1+\cdots+S_f$, such that it is invariant under one supergroup of **L**. In other words **L** is the maximal line group under which S is invariant. This implies that S contains one of the minimal combinations[1] of the orbits of **L**. Table I enables one to find these combinations. In fact, the monomer of S is the union $Y=Y_1+\cdots+Y_f$ of the monomers of the orbits contained in S. If Y is invariant under some supergroup **P**′ of **P**, such that **ZP**′ is a line group, being a supergroup of **L** and leaving S invariant, obviously S is not a minimal

TABLE VII. Vibrational representations of the orbits of the line groups **L**nmm and **L**nm; $n=1,2,\ldots$; translational period is 1 unit. Summation is performed over $k\in(-\pi,\pi]$, $m\in(0,n/2)$. $c=\rho\cos(\pi/n)$ and $s=\rho\sin(\pi/n)$. Orbit c_1 exists for n even, only. Minimal sets: $2a$, $2b$, $2c$, $a+b$, $a+c$, $a+d$, $b+c$, $b+d$, or $c+d$.

Orbit	Orbit point	Vibrational representation
a_1 n even	(x,y,z)	$3\sum_k({}_kA_o + {}_kB_o) + 6\sum_{k,m}{}_kE_{m,-m}+$ $+3\sum_k({}_kA_{n/2} + {}_kB_{n/2})$
b_1 n even	$(x,0,z)$	$\sum_k(2{}_kA_o + {}_kB_o) + 3\sum_{k,m}{}_kE_{m,-m}+$ $+\sum_k(2{}_kA_{n/2} + {}_kB_{n/2})$
c_1	(c,s,z)	$\sum_k[2({}_kA_o + {}_kB_{n/2}) + {}_kB_o + {}_kA_{n/2})] + 3\sum_{k,m}{}_kE_{m,-m}$
d_1	$(0,0,z)$	$\sum_k(2{}_kA_o + {}_kB_o)$; $n=1$ $\sum_k({}_kA_o + {}_kA_1 + {}_kB_1)$; $n=2$ $\sum_k({}_kA_o + {}_kE_{1,-1})$; $n>2$

TABLE VIII. Vibrational representations of the orbits of the line groups **L**ncc and **L**nc $n=1,2,\ldots$; translational period is 1 unit. Summation is performed over $k\in(-\pi,\pi]$, $m\in(0,n/2)$. Minimal sets: $2a$.

Orbit	Orbit point	Vibrational representation
a_1 n even	(x,y,z)	$3\sum_k({}_kA_o + {}_kB_o) + 6\sum_{k,m}{}_kE_{m,-m}+$ $+3\sum_k({}_kA_{n/2} + {}_kB_{n/2})$
b_1	$(0,0,z)$	$3\sum_k({}_kA_o + {}_kB_o)$; $n=1$ $\sum_k[{}_kA_o + {}_kB_o + 2({}_kA_1 + {}_kB_1)]$; $n=2$ $\sum_k[{}_kA_o + {}_kB_o + 2{}_kE_{1,-1}]$; $n>2$

TABLE IX. Vibrational representations of the orbits of the line groups $\mathbf{L}(2n)_n mc$ $n=1,2,\dots$; translational period is 1 unit. Summation is performed over $k\in(-\pi,\pi]$, $m\in(0,n)$. Minimal sets: $2a$, $2b$, $a+b$, $a+d$, or $b+d$.

Orbit	Orbit point	Vibrational representation
a_1	(x,y,z)	$3\sum_k({}_kA_o + {}_kB_o + {}_kA_n + {}_kB_n) + 6\sum_{k,m}{}_kE_{m,-m}$
b_1	$(x,0,z)$	$\sum_k[2({}_kA_o + {}_kA_n) + {}_kB_o + {}_kB_n] + 3\sum_{k,m}{}_kE_{m,-m}$
d_1	$(0,0,z)$	$\sum_k[2({}_kA_o + {}_kA_1) + {}_kB_o + {}_kB_1];\ n=1$ $\sum_k({}_kA_o + {}_kA_n + {}_kE_{n-1,-n+1} + {}_kE_{1,-1});\ n>1$

set for **L**. Hence, given an orbit of **L**, the maximal axial point group of the monomer, $\mathbf{P}_M$, can be easily found (column 5 of Table I). Then, the symmetry of the orbit is $\mathbf{P}'\mathbf{Z}$, where $\mathbf{P}'$ is the maximal subgroup of $\mathbf{P}_M$ which can be combined with **Z** (i.e., commutes with **Z**). This subgroup is $\mathbf{P}_M$ itself if $\mathbf{Z}=\mathbf{T},\mathbf{T}_c,(\mathbf{2n})_1$, because each point group can be combined with them (no "Not group" labels in the corresponding columns). Consequently, for these groups the minimal combinations of the orbits are just as for the point groups in the sense that if in the minimal set for the point group (e.g., $2a+b+\cdots$) any possible combination of indices is inserted ($a_\alpha+a_\beta+b_\gamma+\cdots$), the minimal set for the line group is obtained. The same is valid for the groups $\mathbf{q}_r\mathbf{C}_n$, but for $\mathbf{q}_r\mathbf{D}_n$ $[\mathbf{q}_r\neq\mathbf{T},(\mathbf{2n})_1]$ the mentioned compatibility condition provides the orbits b and c are minimal, because $\mathbf{D}_{nh}$ (precisely σ_v) is not compatible with the screw axis. The minimal sets are given in the captions of Tables II–XIV.

Since the irreducible components of the symmetrized squares of the real representations of the line groups have been published recently, it remains to construct the representations $S^V(\mathbf{L})$ of the minimal sets utilizing Tables II–XIV. Then the translational and rotational modes should be subtracted. The translational modes are contained in the polar-vector representation. As for rotations, it should be noticed that the stereoregular polymer is infinite along the z axis, but finite in other dimensions. This means that only rotations around the z axis are considered.[12] Therefore, the vibrational representation is obtained by the subtraction of the polar-vector and z component of the axial-vector representation[11] (the results for the groups $\mathbf{L}q_p$, $\mathbf{L}q_p2$, $\mathbf{L}q_p22$ are given in the Appendix) from the dynamical representation. Finally, comparing the vibrational representations of the minimal sets with the known symmetrized squares[4] of the real representations verifies the Jahn-Teller theorem for the polymers.

TABLE X. Vibrational representations of the orbits of the line groups $\mathbf{L}(\overline{2n})2m$, and $\mathbf{L}\bar{n}m$, $n=1,2,\dots$; translational period is 1 unit. Summation is performed over $k\in(0,\pi)$, $m\in(0,n/2)$. $c=\rho\cos(\pi/2n)$ and $s=\rho\sin(\pi/2n)$. Minimal sets: a, b, or c.

Orbit	Orbit point	Vibrational representation
a_1	(x,y,z)	$3({}_oA_o^+ + {}_oA_o^- + {}_oB_o^+ + {}_oB_o^- + {}_\pi A_o^+ + {}_\pi A_o^- + {}_\pi B_o^+ + {}_\pi B_o^-)+$ $+6\sum_m({}_oE^+_{m,-m} + {}_oE^-_{m,-m} + {}_\pi E^+_{m,-m} + {}_\pi E^-_{m,-m}) + 6\sum_k({}_k^{-k}E_{A_o} + {}_k^{-k}E_{B_o}) + 12\sum_{k,m}{}_k^{-k}G_{m,-m}+$
n even		$+6({}_oE_{n/2} + {}_\pi E_{n/2}) + 6\sum_k({}_k^{-k}E^{A_{n/2}}_{B_{n/2}} + {}_k^{-k}E^{B_{n/2}}_{A_{n/2}})$
a_2	$(c,s,\frac{1}{2})$	${}_oA_o^+ + {}_oB_o^+ + {}_\pi A_o^- + {}_\pi B_o^- + 2({}_oA_o^- + {}_oB_o^- + {}_\pi A_o^+ + {}_\pi B_o^+)+$ $+3\sum_m({}_oE^+_{m,-m} + {}_oE^-_{m,-m} + {}_\pi E^+_{m,-m} + {}_\pi E^-_{m,-m}) + 3\sum_k({}_k^{-k}E_{A_o} + {}_k^{-k}E_{B_o}) + 6\sum_{k,m}{}_k^{-k}G_{m,-m}+$
n even		$+3({}_oE_{n/2} + {}_\pi E_{n/2}) + 3\sum_k({}_k^{-k}E^{A_{n/2}}_{B_{n/2}} + {}_k^{-k}E^{B_{n/2}}_{A_{n/2}})$
b_1	$(x,0,z)$	$2({}_oA_o^+ + {}_oA_o^- + {}_\pi A_o^+ + {}_\pi A_o^-) + {}_\pi B_o^+ + {}_\pi B_o^- + {}_oB_o^+ + {}_oB_o^- +$ $+3\sum_m({}_oE^+_{m,-m} + {}_oE^-_{m,-m} + {}_\pi E^+_{m,-m} + {}_\pi E^-_{m,-m}) + \sum_k(4{}_k^{-k}E_{A_o} + 2{}_k^{-k}E_{B_o}) + 6\sum_{k,m}{}_k^{-k}G_{m,-m}+$
n even		$+3({}_oE_{n/2} + {}_\pi E_{n/2}) + 3\sum_k 3({}_k^{-k}E^{A_{n/2}}_{B_{n/2}} + {}_k^{-k}E^{B_{n/2}}_{A_{n/2}})$
c_1	$(c,s,0)$	${}_oA_o^+ + {}_oB_o^+ + {}_\pi A_o^+ + {}_\pi B_o^+ + 2({}_oA_o^- + {}_oB_o^- + {}_\pi A_o^- + {}_\pi B_o^-)+$ $+3\sum_m({}_oE^+_{m,-m} + {}_oE^-_{m,-m} + {}_\pi E^+_{m,-m} + {}_\pi E^-_{m,-m}) + 3\sum_k({}_k^{-k}E_{A_o} + {}_k^{-k}E_{B_o}) + 6\sum_{k,m}{}_k^{-k}G_{m,-m}+$
n even		$+3({}_oE_{n/2} + {}_\pi E_{n/2}) + 3\sum_k({}_k^{-k}E^{A_{n/2}}_{B_{n/2}} + {}_k^{-k}E^{B_{n/2}}_{A_{n/2}})$
d_1	$(0,0,z)$	$2({}_oA_o^+ + {}_oA_o^- + {}_\pi A_o^+ + {}_\pi A_o^-) + {}_oB_o^+ + {}_oB_o^- + {}_\pi B_o^+ + {}_\pi B_o^- + \sum_k(4{}_k^{-k}E_{A_o} + 2{}_k^{-k}E_{B_o});\ n=1$ ${}_oA_o^+ + {}_oA_o^- + {}_\pi A_o^+ + {}_\pi A_o^- + 2\sum_k({}_k^{-k}E_{A_o} + {}_k^{-k}E^{A_1}_{B_1} + {}_k^{-k}E^{B_1}_{A_1}) + 2({}_oE_1 + {}_\pi E_1);\ n=2$ ${}_oA_o^+ + {}_oA_o^- + {}_\pi A_o^+ + {}_\pi A_o^- + {}_oE^+_{1,-1} + {}_oE^-_{1,-1} + {}_\pi E^+_{1,-1} + {}_\pi E^-_{1,-1} + 2\sum_k({}_k^{-k}E_{A_o} + {}_k^{-k}G_{1,-1});\ n>2$
d_2	$(0,0,\frac{1}{2})$	$2({}_oA_o^- + {}_\pi A_o^+) + {}_oB_o^+ + {}_\pi B_o^- + \sum_k(2{}_k^{-k}E_{A_o} + {}_k^{-k}E_{B_o});\ n=1$ ${}_oA_o^- + {}_\pi A_o^+ + \sum_k({}_k^{-k}E_{A_o} + {}_k^{-k}E^{A_1}_{B_1} + {}_k^{-k}E^{B_1}_{A_1}) + {}_oE_1 + {}_\pi E_1;\ n=2$ ${}_oA_o^- + {}_\pi A_o^+ + {}_oE^+_{1,-1} + {}_\pi E^-_{1,-1} + \sum_k({}_k^{-k}E_{A_o} + {}_k^{-k}G_{1,-1});\ n>2$
e_1	$(0,0,0)$	$2({}_oA_o^- + {}_\pi A_o^-) + {}_oB_o^+ + {}_\pi B_o^+ + \sum_k(2{}_k^{-k}E_{A_o} + {}_k^{-k}E_{B_o});\ n=1$ ${}_oA_o^- + {}_\pi A_o^- + \sum_k({}_k^{-k}E_{A_o} + {}_k^{-k}E^{A_1}_{B_1} + {}_k^{-k}E^{B_1}_{A_1}) + {}_oE_1 + {}_\pi E_1;\ n=2$ ${}_oA_o^- + {}_\pi A_o^- + {}_oE^+_{1,-1} + {}_\pi E^+_{1,-1} + \sum_k({}_k^{-k}E_{A_o} + {}_k^{-k}G_{1,-1});\ n>2$

TABLE XI. Vibrational representations of the orbits of the line groups $\mathbf{L}(\overline{2n})2c$ and $\mathbf{L}\bar{n}c$; $n=1,2,\ldots$; translational period is 1 unit. Summation is performed over $k \in (0,\pi)$, $m \in (0,n/2)$. Orbit a_2 exists for n odd, only. Minimal sets: $2a$ for n even and a for n odd.

Orbit	Orbit point	Vibrational representation
a_1 n even	(x,y,z)	$3({}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^-) + 6{}_\pi E_0 + 6\sum_m({}_0E_{m,-m}^+ + {}_0E_{m,-m}^- + {}_\pi E_{m,-m}^+ + {}_\pi E_{m,-m}^-)+$ $+6\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0}) + 12\sum_{k,m}{}_k^{-k}G_{m,-m}+$ $+3({}_\pi A_{n/2}^+ + {}_\pi A_{n/2}^- + {}_\pi B_{n/2}^+ + {}_\pi B_{n/2}^-) + 6{}_0E_{n/2} + 6\sum_k({}_k^{-k}E_{B_{n/2}}^{A_{n/2}} + {}_k^{-k}E_{A_{n/2}}^{B_{n/2}})$
a_2	$(0,y,\frac{1}{4})$	${}_0A_0^+ + {}_0B_0^+ + 2({}_0B_0^- + {}_0A_0^-) + 3{}_\pi E_0 + 3\sum_m({}_0E_{m,-m}^+ + {}_0E_{m,-m}^- + {}_\pi E_{m,-m}^+ + {}_\pi E_{m,-m}^-)+$ $+3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0}) + 6\sum_{k,m}{}_k^{-k}G_{m,-m}$
b_1	$(0,0,z)$	$3({}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^-) + 6{}_\pi E_0 + 6\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0});\ n=1$ ${}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^- + 2({}_\pi E_0 + {}_\pi A_1^+ + {}_\pi A_1^- + {}_\pi B_1^+ + {}_\pi B_1^-) + 4{}_0E_1+$ $+\sum_k[4({}_k^{-k}E_{B_1}^{A_1} + {}_k^{-k}E_{A_1}^{B_1}) + 2({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0})];\ n=2$ ${}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^- + 2({}_\pi E_0 + {}_0E_{1,-1}^+ + {}_0E_{1,-1}^- + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^-)+$ $+\sum_k[4{}_k^{-k}G_{1,-1} + 2({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0})];\ n>2$
b_2	$(0,0,\frac{1}{4})$	${}_0A_0^+ + {}_0B_0^+ + 2({}_0A_0^- + {}_0B_0^-) + 3{}_\pi E_0 + 3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0});\ n=1$ ${}_0A_0^- + {}_0B_0^- + {}_\pi E_0 + {}_\pi A_1^+ + {}_\pi A_1^- + {}_\pi B_1^+ + {}_\pi B_1^- + 2{}_0E_1+$ $+\sum_k[2({}_k^{-k}E_{B_1}^{A_1} + {}_k^{-k}E_{A_1}^{B_1}) + {}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0}];\ n=2$ ${}_0A_0^- + {}_0B_0^- + {}_\pi E_0 + {}_0E_{1,-1}^+ + {}_0E_{1,-1}^- + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^- + \sum_k(2{}_k^{-k}G_{1,-1} + {}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0});\ n>2$
c_1	$(0,0,0)$	$3({}_0A_0^- + {}_0B_0^+) + 3{}_\pi E_0 + 3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0});\ n=1$ ${}_0A_0^- + {}_0B_0^+ + {}_\pi E_0 + {}_\pi A_1^+ + {}_\pi A_1^- + {}_\pi B_1^+ + {}_\pi B_1^- + 2{}_0E_1+$ $+\sum_k[2({}_k^{-k}E_{B_1}^{A_1} + {}_k^{-k}E_{A_1}^{B_1}) + {}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0}];\ n=2$ ${}_0A_0^- + {}_0B_0^+ + {}_\pi E_0 + 2{}_0E_{1,-1}^+ + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^- + \sum_k(2{}_k^{-k}G_{1,-1} + {}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0});\ n>2$

V. DISCUSSION

The line-group factorization is used in order to find the orbits of the stereoregular polymers. It has been shown that the line- and point-group orbits are closely related. Further, the minimal sets of orbits, which determine the symmetry of the polymer, are given. The dynamical representation for all orbits of the line groups is reduced to its irreducible components, with the help of the induction procedure, i.e., the symmetry classification of all possible normal vibrations is found. Afterward, the Jahn-Teller theorem for the polymers is proved. All the results are checked numerically (a program dealing with the line groups and applications in polymer physics is in preparation).

In order to determine the exact form of the normal displacements of the concrete system, the group-projector technique[10,2] should be used. As for the single orbit S with the monomer Y, the induction method gives the general expression; note that the group projector of the μth irreducible (n_μ-dimensional) representation is an infinite matrix, with $3|Y|$-dimensional blocks:

$$[S_s^{V(\mu)}]_{ij} = \frac{n_\mu}{|\mathbf{L}|}\sum_l d_{s1}^{(\mu)*}(z^i l z^{-j}) Y^V(l) . \tag{5}$$

Here, the summation is as in (4), over the symmetry group of the monomer; block indices i and j essentially denumerate monomers, s refers to the rows of the representation μ, while $Y^V(l)$ is the dynamical representation of the monomer. As usual, the group projector is obtained for $s=1$, and its eigenvectors for the eigenvalue 1 give the basis for the first row of the μth representation, and the rest of the μth modes are obtained by acting on this basis by the operators $S_s^{(\mu)}$ for $s=2,3,\ldots,n_\mu$.

According to (4), there are a_μ normal modes corresponding to μth representation, and for $a_\mu > 1$, the group-projector technique gives only the subspace of their linear combinations. The exact displacements can be found only by the diagonalization of the vibrational Hamiltonian in this subspace, i.e., the parameters of the concrete system (configuration, force constants) are involved. Analogously, if the polymer contains more than one orbit $S_1+S_2+\cdots+S_k$, the corresponding projectors are $S_s^{V(\mu)} = \oplus_{i=1}^{k} S_{si}^{V(\mu)}$. If an irreducible representation occurs in different orbits, polymer normal displacements for this representation are linear combinations of the orbital ones, and cannot be determined by symmetry arguments only.

For instance, *trans*-polyacetylene $(\mathrm{CH})_x$, with the symmetry group $\mathbf{L}2_1/mcm$, consists of two e_1-type orbits, one for each sort of atoms (Fig. 1). Among its normal coordinates there is one corresponding to the irreducible representation $\mu = {}_0A_1^-$ (also denoted by[13] B_{2g}). The polymer group projector is $e_{1C}^{V(\mu)} \oplus e_{1H}^{V(\mu)}$. The stabilizer of the orbit e_1 is $\mathbf{D}_{1h} = \{e, \sigma_{xz}, \sigma_h, U_x\}$ (Table I). The matrices of the monomer dynamical representation of $\mathbf{D}_{1h}$ are those of the polar-vector representation. Noticing that the generator of $\mathbf{Z}$ is $(C_2|\frac{1}{2})$, (5) reads

$$[e_1^{V(\mu)}]_{ij} = \frac{(-1)^{i+j}}{|\mathbf{Z}|}\begin{bmatrix}0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 1\end{bmatrix}.$$

Normal displacements, obtained with this projector are $x_i = y_i = 0$, and $z_i = (-1)^i z_0$, i.e., the mode is alternating, distortive, and longitudinal. For each orbit (C and H), there is such a mode, and polyacetylene normal modes are combinations of them (Fig. 1).

The possibility of the cooperative vibronic instability in *trans*-polyacetylene (uniform bond length) yielding the distorted *trans-transoid* isomer (alternating bond length)

TABLE XII. Vibrational representations of the orbits of the line groups $\mathbf{L}n/mmm$ and $\mathbf{L}(\overline{2n})2m$; $n = 1, 2, \ldots$; translational period is 1 unit. Summation is performed over $k \in (0, \pi)$, $m \in (0, n/2)$. $c = \rho\cos(\pi/n)$ and $s = \rho\sin(\pi/n)$. Orbits c_1, c_2, and f_1 exist for n even, only. Minimal sets: a, b, c, d, e, or f.

Orbit	Orbit point	Vibrational representation
a_1	(x,y,z)	$3({}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^- + {}_\pi A_0^+ + {}_\pi A_0^- + {}_\pi B_0^+ + {}_\pi B_0^-) + 6\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0}) +$ $+6\sum_m({}_\pi E_{m,-m}^+ + {}_\pi E_{m,-m}^- + {}_0E_{m,-m}^+ + {}_0E_{m,-m}^-) + 12\sum_{k,m}{}_k^{-k}G_{m,-m} +$
n even		$+3({}_0A_{n/2}^+ + {}_0A_{n/2}^- + {}_0B_{n/2}^+ + {}_0B_{n/2}^- + {}_\pi A_{n/2}^+ + {}_\pi A_{n/2}^- + {}_\pi B_{n/2}^+ + {}_\pi B_{n/2}^-) + 6\sum_k({}_k^{-k}E_{A_{n/2}} + {}_k^{-k}E_{B_{n/2}})$
a_2	$(x,y,\frac{1}{2})$	$2({}_0A_0^+ + {}_0B_0^+ + {}_\pi A_0^- + {}_\pi B_0^-) + {}_0A_0^- + {}_0B_0^- + {}_\pi A_0^+ + {}_\pi B_0^+ + 3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0}) +$ $+\sum_m[4({}_\pi E_{m,-m}^- + {}_0E_{m,-m}^+) + 2({}_\pi E_{m,-m}^+ + {}_0E_{m,-m}^-)] + 6\sum_{k,m}{}_k^{-k}G_{m,-m} +$
n even		$+2({}_0A_{n/2}^+ + {}_0B_{n/2}^+ + {}_\pi A_{n/2}^- + {}_\pi B_{n/2}^-) + {}_0A_{n/2}^- + {}_0B_{n/2}^- + {}_\pi A_{n/2}^+ + {}_\pi B_{n/2}^+ + 3\sum_k({}_k^{-k}E_{A_{n/2}} + {}_k^{-k}E_{B_{n/2}})$
b_1	$(x,0,z)$	$2({}_0A_0^+ + {}_0A_0^- + + {}_\pi A_0^+ + {}_\pi A_0^-) + {}_0B_0^+ + {}_0B_0^- + {}_\pi B_0^+ + {}_\pi B_0^- + 6\sum_{k,m}{}_k^{-k}G_{m,-m} +$ $+\sum_k(2{}_k^{-k}E_{B_0} + 4{}_k^{-k}E_{A_0}) + 3\sum_m({}_\pi E_{m,-m}^+ + {}_\pi E_{m,-m}^- + {}_0E_{m,-m}^+ + {}_0E_{m,-m}^-)$
n even		$+2({}_0A_{n/2}^+ + {}_0A_{n/2}^- + {}_\pi A_{n/2}^+ + {}_\pi A_{n/2}^-) + {}_0B_{n/2}^+ + {}_0B_{n/2}^- + {}_\pi B_{n/2}^+ + {}_\pi B_{n/2}^- + \sum_k(2{}_k^{-k}E_{B_{n/2}} + 4{}_k^{-k}E_{A_{n/2}})$
b_2	$(x,0,\frac{1}{2})$	${}_0A_0^+ + {}_0A_0^- + {}_\pi A_0^- + {}_\pi A_0^+ + {}_0B_0^+ + {}_\pi B_0^- + \sum_k({}_k^{-k}E_{B_0} + 2{}_k^{-k}E_{A_0}) +$ $+\sum_m[2({}_\pi E_{m,-m}^- + {}_0E_{m,-m}^+) + {}_\pi E_{m,-m}^+ + {}_0E_{m,-m}^-] + 3\sum_{k,m}{}_k^{-k}G_{m,-m} +$
n even		$+{}_0A_{n/2}^+ + {}_0A_{n/2}^- + {}_\pi A_{n/2}^- + {}_\pi A_{n/2}^+ + {}_0B_{n/2}^+ + {}_\pi B_{n/2}^- + \sum_k({}_k^{-k}E_{B_{n/2}} + 2{}_k^{-k}E_{A_{n/2}})$
c_1	(c,s,z)	$2({}_0A_0^+ + {}_0A_0^- + {}_0B_{n/2}^+ + {}_0B_{n/2}^- + {}_\pi B_{n/2}^+ + {}_\pi B_{n/2}^- + {}_\pi A_0^+ + {}_\pi A_0^-) + {}_0B_0^+ + {}_0B_0^- + {}_0A_{n/2}^+ + {}_0A_{n/2}^- +$ $+{}_\pi B_0^+ + {}_\pi B_0^- + {}_\pi A_{n/2}^+ + {}_\pi A_{n/2}^- + \sum_k[2({}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_{n/2}}) + 4({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_{n/2}})] +$ $+3\sum_m({}_\pi E_{m,-m}^+ + {}_\pi E_{m,-m}^- + {}_0E_{m,-m}^+ + {}_0E_{m,-m}^-) + 6\sum_{k,m}{}_k^{-k}G_{m,-m}$
c_2	$(c,s,\frac{1}{2})$	${}_0A_0^- + {}_0B_{n/2}^+ + {}_0B_{n/2}^- + {}_\pi B_{n/2}^+ + {}_\pi B_{n/2}^- + {}_\pi A_0^+ + {}_\pi A_0^- + {}_0B_0^+ + {}_0A_{n/2}^+ + {}_\pi B_0^- + {}_\pi A_{n/2}^- + 3\sum_{k,m}{}_k^{-k}G_{m,-m} +$ $+\sum_k[{}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_{n/2}} + 2({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_{n/2}})] + \sum_m[2({}_\pi E_{m,-m}^- + {}_0E_{m,-m}^+) + {}_\pi E_{m,-m}^+ + {}_0E_{m,-m}^-] + {}_0A_0^+$
d_1	$(x,y,0)$	$2({}_0A_0^+ + {}_0B_0^+ + {}_\pi A_0^+ + {}_\pi B_0^+) + {}_0A_0^- + {}_0B_0^- + {}_\pi A_0^- + {}_\pi B_0^- +$ $+3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0}) + \sum_m[4({}_\pi E_{m,-m}^+ + {}_0E_{m,-m}^+) + 2({}_\pi E_{m,-m}^- + {}_0E_{m,-m}^-)] + 6\sum_{k,m}{}_k^{-k}G_{m,-m} +$
n even		$+2({}_\pi A_{n/2}^+ + {}_\pi B_{n/2}^+ + {}_0A_{n/2}^+ + {}_0B_{n/2}^+) + {}_\pi A_{n/2}^- + {}_\pi B_{n/2}^- + {}_0A_{n/2}^- + {}_0B_{n/2}^- + 3\sum_k({}_k^{-k}E_{A_{n/2}} + {}_k^{-k}E_{B_{n/2}})$
e_1	$(x,0,0)$	${}_0A_0^+ + {}_0A_0^- + {}_\pi A_0^+ + {}_\pi A_0^- + {}_0B_0^+ + {}_\pi B_0^+ + \sum_k({}_k^{-k}E_{B_0} + 2{}_k^{-k}E_{A_0}) + 3\sum_{k,m}{}_k^{-k}G_{m,-m} +$ $+\sum_m[2({}_\pi E_{m,-m}^+ + {}_0E_{m,-m}^+) + {}_\pi E_{m,-m}^- + {}_0E_{m,-m}^-] +$
n even		$+{}_0A_{n/2}^+ + {}_0A_{n/2}^- + {}_\pi A_{n/2}^+ + {}_\pi A_{n/2}^- + {}_0B_{n/2}^+ + {}_\pi B_{n/2}^+ + \sum_k({}_k^{-k}E_{B_{n/2}} + 2{}_k^{-k}E_{A_{n/2}})$
f_1	$(c,s,0)$	${}_0A_0^- + {}_0B_{n/2}^+ + {}_0B_{n/2}^- + {}_\pi B_{n/2}^+ + {}_\pi B_{n/2}^- + {}_\pi A_0^+ + {}_\pi A_0^- + {}_0B_0^+ + {}_0A_{n/2}^+ + {}_\pi B_0^+ + {}_\pi A_{n/2}^+ + 3\sum_{k,m}{}_k^{-k}G_{m,-m} +$ $+\sum_k[{}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_{n/2}} + 2({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_{n/2}})] + \sum_m[2({}_\pi E_{m,-m}^+ + {}_0E_{m,-m}^+) + {}_\pi E_{m,-m}^- + {}_0E_{m,-m}^-] + {}_0A_0^+$
g_1	$(0,0,z)$	$2({}_0A_0^+ + {}_0A_0^- + {}_\pi A_0^+ + {}_\pi A_0^-) + {}_0B_0^+ + {}_0B_0^- + {}_\pi B_0^+ + {}_\pi B_0^- + \sum_k(4{}_k^{-k}E_{A_0} + 2{}_k^{-k}E_{B_0});\ n = 1$ ${}_0A_0^- + {}_0A_0^+ + {}_\pi A_0^- + {}_\pi A_0^+ + {}_0A_1^+ + {}_0A_1^- + {}_\pi A_1^+ + {}_\pi A_1^- + {}_0B_1^+ + {}_0B_1^- + {}_\pi B_1^+ + {}_\pi B_1^- +$ $+2\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_1} + {}_k^{-k}E_{B_1});\ n = 2$ ${}_0A_0^+ + {}_0A_0^- + {}_\pi A_0^+ + {}_\pi A_0^- + {}_0E_{1,-1}^+ + {}_0E_{1,-1}^- + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^- + 2\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}G_{1,-1});\ n > 2$
g_2	$(0,0,\frac{1}{2})$	${}_0A_0^+ + {}_0A_0^- + {}_\pi A_0^+ + {}_\pi A_0^- + {}_0B_0^+ + {}_\pi B_0^- + \sum_k(2{}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0});\ n = 1$ ${}_0A_0^- + {}_\pi A_0^+ + {}_0A_1^+ + {}_\pi A_1^- + {}_0B_1^+ + {}_\pi B_1^- + \sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_1} + {}_k^{-k}E_{B_1});\ n = 2$ ${}_0A_0^- + {}_\pi A_0^+ + {}_0E_{1,-1}^+ + {}_\pi E_{1,-1}^- + \sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}G_{1,-1});\ n > 2$
h_1	$(0,0,0)$	${}_0A_0^+ + {}_0A_0^- + {}_\pi A_0^+ + {}_\pi A_0^- + {}_0B_0^+ + {}_\pi B_0^+ + \sum_k(2{}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0});\ n = 1$ ${}_0A_0^- + {}_\pi A_0^- + {}_0A_1^+ + {}_\pi A_1^+ + {}_0B_1^+ + {}_\pi B_1^+ + \sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_1} + {}_k^{-k}E_{B_1});\ n = 2$ ${}_0A_0^- + {}_\pi A_0^- + {}_0E_{1,-1}^+ + {}_\pi E_{1,-1}^+ + \sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}G_{1,-1});\ n > 2$

is frequently discussed in the literature.[13,14] The following symmetry analysis confirms such claims. At first, from the table[6] of the representations of the group $\mathbf{L}2_1/mcm$ it is obvious that there can be at most four types of the π-electron energy bands: ${}_kE_{A_0}$, ${}_kE_{A_1}$, ${}_kE_{B_0}$, and ${}_kE_{B_1}$. Compatibility relations[10,2] at $k=\pi$ stick together the bands ${}_kE_{A_0}$ and ${}_kE_{A_1}$, as well as the bands ${}_kE_{B_0}$ and ${}_kE_{B_1}$ (Fig. 2). There is one electron per monomer, i.e., two electrons per translational unit cell, and the Fermi radius equals π.

On the other side, the Hückel's π-electron theory, using the p_y atomic orbitals, gives the B_1^+ representation of the point group $\mathbf{D}_{2h}$ for the bonding π_u orbital in the C-C bond.[13] Hence, the corresponding polymer orbital transforms according to the representation

$$e_1(\mathbf{L}2_1/mcm)\otimes {}_0B_1^+(\mathbf{L}2_1/mcm)$$
$$={}_0B_0^+ + {}_0B_1^+ + {}_kE_{B_0} + {}_kE_{B_1} + {}_\pi E_B \;.$$

This implies that the relevant electronic state at the Fermi level is ${}_\pi E_B$, connecting the bands ${}_kE_{B_0}$ and ${}_kE_{B_1}$ (Fig. 2). So, the band is half-filled and in the ground state *trans*-polyacetylene is an intrinsic metal with degenerate ground state. This is the classical situation of the cooperative Jahn-Teller vibronic instability. The candidates for the symmetry of the soft mode are the irreducible components of the symmetrized square $[{}_\pi E_B^2]={}_0A_0^+ + {}_0A_1^+ + {}_0A_1^-$, which are all contained in the dynamical representation for the orbit of C-ions

$$e_1^V={}_0A_0^+ + {}_0A_0^- + {}_0A_1^+ + {}_0A_1^- + {}_0B_0^+ + {}_0B_1^+ + 2\,{}_\pi E_A + {}_\pi E_B + \sum_k [{}_{\bar{k}}^{k}E_{B_0} + {}_{\bar{k}}^{k}E_{B_1} + 2({}_{\bar{k}}^{k}E_{A_0} + {}_{\bar{k}}^{k}E_{A_1})]$$

TABLE XIII. Vibrational representations of the orbits of the line groups $\mathbf{L}n/mcc$ and $\mathbf{L}(\overline{2n})2c$; $n=1,2,\ldots$; translational period is 1 unit. Summation is performed over $k\in(0,\pi)$, $m\in(0,n/2)$. Orbit a_3 exists for $n=4p+2$, $(p=0,1,\ldots)$ only. Minimal sets: $2a$, $2b$, or $a+b$.

Orbit	Orbit point	Vibrational representation
a_1 n even	(x,y,z)	$3({}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^-) + 6{}_\pi E_0 + 6\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0})+$ $+6\sum_m({}_\pi E_{m,-m}^+ + {}_\pi E_{m,-m}^- + {}_0E_{m,-m}^+ + {}_0E_{m,-m}^-) + 12\sum_{k,m}{}_k^{-k}G_{m,-m}+$ $+3({}_0A_{n/2}^+ + {}_0A_{n/2}^- + {}_0B_{n/2}^+ + {}_0B_{n/2}^-) + 6{}_\pi E_{n/2} + 6\sum_k({}_k^{-k}E_{A_{n/2}} + {}_k^{-k}E_{B_{n/2}})$
a_2 n even	$(x,0,\frac{1}{4})$	$2({}_0A_0^- + {}_0B_0^+) + {}_0A_0^+ + {}_0B_0^- + 3{}_\pi E_0 + 3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0}) + 6\sum_{k,m}{}_k^{-k}G_{m,-m}+$ $+3\sum_m({}_\pi E_{m,-m}^+ + {}_\pi E_{m,-m}^- + {}_0E_{m,-m}^+ + {}_0E_{m,-m}^-)+$ $+2({}_0A_{n/2}^- + {}_0B_{n/2}^+) + {}_0A_{n/2}^+ + {}_0B_{n/2}^- + 3{}_\pi E_{n/2} + 3\sum_k({}_k^{-k}E_{A_{n/2}} + {}_k^{-k}E_{B_{n/2}})$
a_3	$(0,y,\frac{1}{4})$	$2({}_0A_0^- + {}_0B_{n/2}^- + {}_0B_0^+ + {}_0A_{n/2}^+) + {}_0A_0^+ + {}_0B_{n/2}^+ + {}_0B_0^- + {}_0A_{n/2}^- + 3({}_\pi E_0 + {}_\pi E_{n/2}) + 6\sum_{k,m}{}_k^{-k}G_{m,-m}+$ $+3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_{n/2}} + {}_k^{-k}E_{B_0} + {}_k^{-k}E_{B_{n/2}}) + 3\sum_m({}_\pi E_{m,-m}^+ + {}_\pi E_{m,-m}^- + {}_0E_{m,-m}^+ + {}_0E_{m,-m}^-)$
b_1 n even	$(x,y,0)$	$2({}_0A_0^+ + {}_0B_0^+) + {}_0A_0^- + {}_0B_0^- + 3{}_\pi E_0 + 3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0})+$ $+\sum_m[3({}_\pi E_{m,-m}^+ + {}_\pi E_{m,-m}^-) + 4{}_0E_{m,-m}^+ + 2{}_0E_{m,-m}^-] + 6\sum_{k,m}{}_k^{-k}G_{m,-m}+$ $+2({}_0A_{n/2}^+ + {}_0B_{n/2}^+) + {}_0A_{n/2}^- + {}_0B_{n/2}^- + 3{}_\pi E_{n/2} + 3\sum_k({}_k^{-k}E_{A_{n/2}} + {}_k^{-k}E_{B_{n/2}})$
c_1	$(0,0,z)$	$3({}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^-) + 6{}_\pi E_0 + 6\sum_k({}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_0})$; $n=1$ ${}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^- + 2({}_0A_1^+ + {}_0A_1^- + {}_0B_1^+ + {}_0B_1^-) + 2{}_\pi E_0 + 4{}_\pi E_1+$ $+\sum_k[2({}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_0}) + 4({}_k^{-k}E_{A_1} + {}_k^{-k}E_{B_1})]$; $n=2$ ${}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^- + 2({}_\pi E_0 + {}_0E_{1,-1}^+ + {}_0E_{1,-1}^- + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^-)+$ $+\sum_k[2({}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_0}) + 4{}_k^{-k}G_{1,-1}]$; $n>2$
c_2	$(0,0,\frac{1}{4})$	$2({}_0A_0^- + {}_0B_0^+) + {}_0A_0^+ + {}_0B_0^- + 3{}_\pi E_0 + 3\sum_k({}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_0})$; $n=1$ ${}_0A_0^- + {}_0B_0^+ + {}_0A_1^+ + {}_0A_1^- + {}_0B_1^+ + {}_0B_1^- + {}_\pi E_0 + 2{}_\pi E_1 + \sum_k[{}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_0} + 2({}_k^{-k}E_{A_1} + {}_k^{-k}E_{B_1})]$; $n=2$ ${}_0A_0^- + {}_0B_0^+ + {}_\pi E_0 + {}_0E_{1,-1}^+ + {}_0E_{1,-1}^- + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^- + \sum_k({}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_0} + 2{}_k^{-k}G_{1,-1})$; $n>2$
d_1	$(0,0,0)$	$2({}_0A_0^+ + {}_0B_0^+) + {}_0A_0^- + {}_0B_0^- + 3{}_\pi E_0 + 3\sum_k({}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_0})$; $n=1$ ${}_0A_0^- + {}_0B_0^- + 2({}_0A_1^+ + {}_0B_1^+) + {}_\pi E_0 + 2{}_\pi E_1 + \sum_k[{}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_0} + 2({}_k^{-k}E_{A_1} + {}_k^{-k}E_{B_1})]$; $n=2$ ${}_0A_0^- + {}_0B_0^- + {}_\pi E_0 + 2{}_0E_{1,-1}^+ + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^- + \sum_k({}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_0} + 2{}_k^{-k}G_{1,-1})$; $n>2$

TABLE XIV. Vibrational representations of the orbits of the line groups $\mathbf{L}(2n)_n/mcm$; $n=1,2,\ldots$; translational period is 1 unit. Summation is performed over $k\in(0,\pi)$. In the primed sums m is from $(0,n/2)$, otherwise from $(0,n)$. $c=\rho\cos(\pi/n)$, $s=\rho\sin(\pi/n)$, $c'=\rho\cos(\pi/2n)$, and $s'=\rho\sin(\pi/2n)$. Orbit f_1 exists for n even, only. Minimal sets: a, b, d, e, or f.

Orbit	Orbit point	Vibrational representation
a_1 n even	(x,y,z)	$3({}_0A_0^+ + {}_0A_0^- + {}_0B_0^+ + {}_0B_0^- + {}_0A_n^+ + {}_0A_n^- + {}_0B_n^+ + {}_0B_n^-) + 12{\sum_m}' {}_\pi G_{m,-m}^{m-n,n-m} + 12\sum_{k,m} {}_k^{-k}G_{m,-m}+$ $+6({}_\pi E_A + {}_\pi E_B) + 6\sum_m({}_0E_{m,-m}^+ + {}_0E_{m,-m}^-) + 6\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_n} + {}_k^{-k}E_{B_n})+$ $+6({}_\pi E_{n/2,-n/2}^+ + {}_\pi E_{n/2,-n/2}^-)$
a_2	$(c',s',\frac{1}{4})$	${}_0A_0^+ + {}_0B_n^+ + {}_0B_0^- + {}_0A_n^- + 2({}_0A_0^- + {}_0B_0^+ + {}_0B_n^- + {}_0A_n^+) + 3({}_\pi E_A + {}_\pi E_B + {}_\pi E_{n/2,-n/2}^+ + {}_\pi E_{n/2,-n/2}^-)+$ $+3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_n} + {}_k^{-k}E_{B_n}) + 3\sum_m({}_0E_{m,-m}^+ + {}_0E_{m,-m}^-) + 6{\sum_m}' {}_\pi G_{m,-m}^{m-n,n-m} + 6\sum_{k,m} {}_k^{-k}G_{m,-m}$
b_1 n even	$(x,0,z)$	$2({}_0A_0^+ + {}_0A_0^- + {}_0A_n^+ + {}_0A_n^- + {}_\pi E_B) + {}_0B_0^+ + {}_0B_0^- + {}_0B_n^+ + {}_0B_n^- + 4{}_\pi E_A + 3\sum_m({}_0E_{m,-m}^+ + {}_0E_{m,-m}^-)+$ $+\sum_k[2({}_k^{-k}E_{B_0} + {}_k^{-k}E_{B_n}) + 4({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_n})] + 6{\sum_m}' {}_\pi G_{m,-m}^{m-n,n-m} + 6\sum_{k,m} {}_k^{-k}G_{m,-m}+$ $+3({}_\pi E_{n/2,-n/2}^+ + {}_\pi E_{n/2,-n/2}^-)$
d_1 n even	$(x,y,0)$	$2({}_0A_0^+ + {}_0B_0^+ + {}_0A_n^+ + {}_0B_n^+) + {}_0A_0^- + {}_0B_0^- + {}_0A_n^- + {}_0B_n^- + 3({}_\pi E_A + {}_\pi E_B) + 6\sum_{k,m} {}_k^{-k}G_{m,-m}$ $+3\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{B_0} + {}_k^{-k}E_{A_n} + {}_k^{-k}E_{B_n}) + \sum_m(4{}_0E_{m,-m}^+ + 2{}_0E_{m,-m}^-) + 6{\sum_m}' {}_\pi G_{m,-m}^{m-n,n-m}+$ $+3({}_\pi E_{n/2,-n/2}^+ + {}_\pi E_{n/2,-n/2}^-)$
e_1 n even	$(x,0,0)$	${}_0A_0^+ + {}_0A_0^- + {}_0A_n^+ + {}_0A_n^- + {}_0B_0^+ + {}_0B_n^+ + 2{}_\pi E_A + {}_\pi E_B + 3{\sum_m}' {}_\pi G_{m,-m}^{m-n,n-m}+$ $+\sum_k[{}_k^{-k}E_{B_0} + {}_k^{-k}E_{B_n} + 2({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_n})] + \sum_m(2{}_0E_{m,-m}^+ + {}_0E_{m,-m}^-) + 3\sum_{k,m} {}_k^{-k}G_{m,-m}+$ $+2{}_\pi E_{n/2,-n/2}^- + {}_\pi E_{n/2,-n/2}^+$
f_1	$(c,s,0)$	${}_0A_0^+ + {}_0A_0^- + {}_0A_n^+ + {}_0B_n^+ + {}_0B_0^+ + {}_0A_n^- + 2({}_\pi E_A + {}_\pi E_{n/2,-n/2}^+) + {}_\pi E_B + {}_\pi E_{n/2,-n/2}^- + 3\sum_{k,m} {}_k^{-k}G_{m,-m}+$ $+\sum_k[{}_k^{-k}E_{B_0} + {}_k^{-k}E_{B_n} + 2({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_n})] + \sum_m(2{}_0E_{m,-m}^+ + {}_0E_{m,-m}^-) + 3{\sum_m}' {}_\pi G_{m,-m}^{m-n,n-m}$
g_1	$(0,0,z)$	$2({}_0A_0^+ + {}_0A_0^- + {}_0A_1^+ + {}_0A_1^- + {}_\pi E_B) + {}_0B_0^+ + {}_0B_0^- + {}_0B_1^+ + {}_0B_1^- + 4{}_\pi E_A+$ $+\sum_k[4({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_1}) + 2({}_k^{-k}E_{B_0} + {}_k^{-k}E_{B_1})]$; $n=1$ ${}_0A_0^+ + {}_0A_0^- + {}_0A_2^+ + {}_0A_2^- + 2({}_\pi E_A + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^- + {}_0E_{1,-1}^+ + {}_0E_{1,-1}^-)+$ $+\sum_k[2({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_2}) + 4{}_k^{-k}G_{1,-1}]$; $n=2$ ${}_0A_0^+ + {}_0A_0^- + {}_0A_n^+ + {}_0A_n^- + 2({}_\pi E_A + {}_\pi G_{1,-1}^{n-1,1-n}) + {}_0E_{1,-1}^+ + {}_0E_{1,-1}^- + {}_0E_{n-1,1-n}^+ + {}_0E_{n-1,1-n}^-+$ $+2\sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_n} + {}_k^{-k}G_{n-1,1-n} + {}_k^{-k}G_{1,-1})$; $n>2$
g_2	$(0,0,\frac{1}{4})$	${}_0A_0^+ + {}_0A_0^- + {}_0A_1^+ + {}_0A_1^- + {}_0B_0^+ + {}_0B_1^- + {}_\pi E_B + 2{}_\pi E_A + \sum_k[2({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_1}) + {}_k^{-k}E_{B_0} + {}_k^{-k}E_{B_1}]$; $n=1$ ${}_0A_0^- + {}_0A_2^+ + {}_\pi E_A + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^- + {}_0E_{1,-1}^+ + {}_0E_{1,-1}^- + \sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_2} + 2{}_k^{-k}G_{1,-1})$; $n=2$ ${}_0A_0^- + {}_0A_n^+ + {}_\pi E_A + {}_0E_{1,-1}^+ + {}_0E_{n-1,1-n}^- + {}_\pi G_{1,-1}^{n-1,1-n} + \sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_n} + {}_k^{-k}G_{n-1,1-n} + {}_k^{-k}G_{1,-1})$; $n>2$
h_1	$(0,0,0)$	${}_0A_0^+ + {}_0A_0^- + {}_0A_1^+ + {}_0A_1^- + {}_0B_0^+ + {}_0B_1^+ + {}_\pi E_B + 2{}_\pi E_A + \sum_k[2({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_1}) + {}_k^{-k}E_{B_0} + {}_k^{-k}E_{B_1}]$; $n=1$ ${}_0A_0^- + {}_0A_2^- + {}_\pi E_A + {}_\pi E_{1,-1}^+ + {}_\pi E_{1,-1}^- + 2{}_0E_{1,-1}^+ + \sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_2} + 2{}_k^{-k}G_{1,-1})$; $n=2$ ${}_0A_0^- + {}_0A_n^- + {}_\pi E_A + {}_0E_{1,-1}^+ + {}_0E_{n-1,1-n}^+ + {}_\pi G_{1,-1}^{n-1,1-n} + \sum_k({}_k^{-k}E_{A_0} + {}_k^{-k}E_{A_n} + {}_k^{-k}G_{n-1,1-n} + {}_k^{-k}G_{1,-1})$; $n>2$

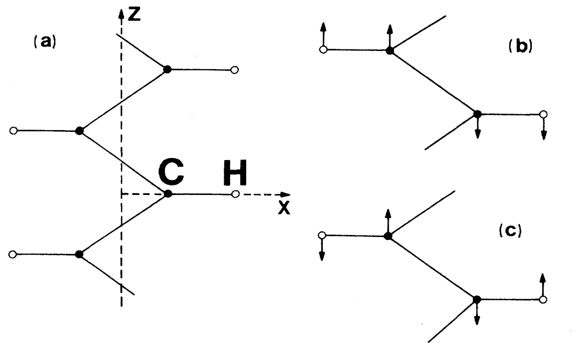

FIG. 1. (a) *trans*-polyacetylene configuration; (b) Jahn-Teller active mode corresponding to ${}_0A_1^-$ irreducible representation; (c) another type of the ${}_0A_1^-$ mode (not active).

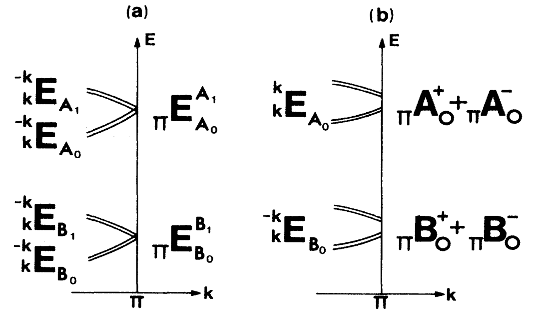

FIG. 2. Band structure at the end of the Brillouin zone (reduced representation is used) of (a) *trans*-polyacetylene and (b) "dimerized" *trans*-polyacetylene.

(Table XIV). After neglecting the totally symmetrical representation and x component of the translations, it remains ${}_0A_1^-$ (Fig. 1), satisfying all the requirements for the Jahn-Teller effect.

If one takes into account both e_1-type orbits the situation is a little bit different. The dynamical representation now becomes $2e_1^V$ and contains ${}_0A_1^-$ twice. The vibrations of the polymer are described by the linear combinations of the independent normal displacements (Fig. 1): atoms from different orbits can oscillate with opposite phase (C-H bending) and in the phase (C-C stretching). For the phase transition the candidate is only the last mode (C-H) bonds are tighter and H ions follow C ions), and the Peierls dimerization occurs. ${}_0A_1^-$ is the representation of the order parameter (soft mode) of the equitranslational structural phase transition. The symmetry predicts[15] $\mathbf{L}\bar{1}m$ for the symmetry group of new configuration. The reflection σ_h is the representative of the "lost" symmetry coset ($\mathbf{L}2_1/mcm=\mathbf{L}\bar{1}m+\sigma_h\mathbf{L}\bar{1}m$), thus restoring the initial symmetry via two possible domains with the soliton[16] in the role of the Goldstone mode.

Both representations ${}_{\bar{k}}^{-k}E_{B_0}$ and ${}_{\bar{k}}^{-k}E_{B_1}$ of $\mathbf{L}2_1/mcm$ subduce into $k_{\bar{k}}^{-k}E_B$ of $\mathbf{L}\bar{1}m$, without any requirement on their connection in $k=\pi$; moreover, in $k=\pi$ this representation reduces into ${}_\pi B_0^+ + {}_\pi B_0^-$. Hence, the energy gains a gap at Fermi level, and the distorted isomer is an intrinsic insulator, with nondegenerate ground state.

In the previous example the order parameter was one dimensional, which is the simplest case. Two- or four-dimensional active modes are possible also (e.g., the representation ${}_\pi G_2$ occurs in the orbit e_1 of the group $\mathbf{L}16_8/mcm$, as well as in the symmetrized square $[{}_{\pi/2}G_1^2]$), giving rise to more complicated, and possibly physically richer phenomena.[4]

Finally, it should be noted again that the above discussion refers to infinite polymers. Finite chains require a somewhat different approach, including considerations imposed by topologically nontrivial Born–von Kármán condition.

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APPENDIX

The irreducible representations of the line groups have been published earlier.[3] Nevertheless, it turns out that some alternative sets of the representations of the families $\mathbf{L}q_p$ and $\mathbf{L}q_p2$, $\mathbf{L}q_p22$ are much more convenient for the purposes of this paper. Therefore these will be derived here, together with some necessary properties. Note that the sets of the irreducible representations for the given group is unique up to equivalence, implying that the alternative sets are essentially the same, but the notation is different due to the different meaning of the quantum numbers involved.

The groups $\mathbf{L}q_p$ are the direct products $\mathbf{q}_r\mathbf{C}_n$, where n is the greatest common divisor of q and p, while r is the unique solution of the equation $rp/q=n \pmod q$ being less than q and coprime relatively to q. Both factors in this product are cyclic groups, generated by $(C_q^r|\xi)$ and $(C_n^s|0)$, respectively, yielding the set of the irreducible representations ($\alpha=2\pi/n$):

$$ {}_kA_m(C_q^{rt}C_n^s|t)=e^{i(kt\xi+ms\alpha)}\ , \quad k\in(-\pi,\pi], $$

$$ m=\begin{cases} -\dfrac{n-1}{2},\dots,\dfrac{n-1}{2}\ , & n \text{ odd}\ , \\ -\dfrac{n-2}{2},\dots,\dfrac{n}{2}\ , & n \text{ even}\ . \end{cases} $$

Complex conjugated representations are ${}_kA_m^*={}_{-k}A_{-m}$, giving rise to the following set of the real irreducible representations: ${}_0A_0$, ${}_\pi A_0$, $({}_kA_m, {}_{-k}A_{-m})={}_kA_m+{}_{-k}A_{-m}$, and only for n even, ${}_0A_{n/2}$, ${}_\pi A_{n/2}$. Symmetrized squares of the two-dimensional representations can be reduced in the form

$$ [({}_kA_m,{}_{-k}A_{-m})^2]={}_\kappa A_\mu+{}_{\kappa'}A_{\mu'}+{}_0A_0\ , $$

with $\kappa\doteq-2k$, $\kappa'\doteq2k$, $\mu\doteq-2m$, and $\mu'\doteq2m$ (here $\doteq$ denotes the equality modulo the range of k and m, respectively). The polar- and axial-vector representations reduce as follows:

$$ V=A=\begin{cases} {}_0A_0+{}_\kappa A_0+{}_{-\kappa}A_0 & n=1\ , \\ {}_0A_0+{}_\kappa A_1+{}_{-\kappa}A_1 & n=2\ , \\ {}_0A_0+{}_\kappa A_1+{}_{-\kappa}A_{-1} & n>2\ , \end{cases} \tag{A1} $$

where κ is equal to $2\pi r/q$ for $2r\le q$ and $2\pi(r/q-1)$ in the opposite case. ${}_0A_0$ corresponds to the z components of translations or rotations, while the remaining irreducible representations belong to the standard linear combinations of the x and y components.[11]

For the groups $\mathbf{L}q_p2,\mathbf{L}q_p22$, being the semidirect product $\mathbf{q}_r\mathbf{D}_n$ of the cyclic invariant subgroup and the dihedral point groups $\mathbf{D}_n$, the induction procedure gives the irreducible representations:

$$ {}_0A_0^\pm(C_q^{rt}U^iC_n^s|t)=(\pm1)^i\ , $$

$$ {}_0E_m^{-m}(C_q^{rt}U^iC_n^s|t)=\begin{bmatrix}0&1\\1&0\end{bmatrix}^i\begin{bmatrix}e^{ims\alpha}&0\\0&e^{-ims\alpha}\end{bmatrix}\ ,\quad m\in\left(0,\frac{n}{2}\right)\ , $$

$$ {}_{\bar{k}}^{-k}E_m^{-m}(C_q^{rt}U^iC_n^s|t)=\begin{bmatrix}0&1\\1&0\end{bmatrix}^i\begin{bmatrix}e^{i(kt\xi+ms\alpha)}&0\\0&e^{-i(kt\xi+ms\alpha)}\end{bmatrix}\ ,\quad k\in(0,\pi),m\in\left(-\frac{n}{2},\frac{n}{2}\right]\ , $$

$$ {}_{\pi}A_0^{\pm}(C_q^{rt}U^iC_n^s|t)=(\pm 1)^i(-1)^t\ , $$

$$ {}_{\pi}E_m^{-m}(C_q^{rt}U^iC_n^s|t)=(-1)^t\begin{bmatrix}0&1\\1&0\end{bmatrix}^i\begin{bmatrix}e^{imsa}&0\\0&e^{-imsa}\end{bmatrix}\ ,\quad m\in\left[0\ ,\frac{n}{2}\right]\ , $$

and only for n even

$$ {}_{0}A_{n/2}^{\pm}(C_q^{rt}U^iC_n^s|t)=(\pm 1)^i(-1)^s\ , $$

$$ {}_{\pi}A_{n/2}^{\pm}(C_q^{rt}U^iC_n^s|t)=(\pm 1)^i(-1)^t(-1)^s\ . $$

All these representations are real, and the symmetrized squares of the two-dimensional representations reduce as follows:

$$
\begin{array}{lll}
[{}_{k}^{-k}E_m^{-m\,2}]= & {}_0A_0^{+}+{}_{2k}^{-2k}E_{\mu}^{-\mu} & k\in\left[0,\frac{\pi}{2}\right]\ ,\ \ \mu\doteq 2m \\
 & {}_0A_0^{+}+{}_{2\pi-2k}^{2k-2\pi}E_{-\mu}^{\mu} & k\in\left[\frac{\pi}{2},\pi\right]\ ,\ \ \mu\doteq 2m \\
 & {}_0A_0^{+}+{}_{\pi}E_{2m+n}^{-2m-n} & k=\frac{\pi}{2}\ ,\ \ m\in\left[-\frac{n}{2}\ ,-\frac{n}{4}\right] \\
 & {}_0A_0^{+}+{}_{\pi}E_{-2m}^{2m} & k=\frac{\pi}{2}\ ,\ \ m\in\left[-\frac{n}{4},0\right] \\
 & {}_0A_0^{+}+{}_{\pi}E_{2m}^{-2m} & k=\frac{\pi}{2}\ ,\ \ m\in\left[0,\frac{n}{4}\right] \\
 & {}_0A_0^{+}+{}_{\pi}E_{-2m+n}^{2m-n} & k=\frac{\pi}{2}\ ,\ \ m\in\left[\frac{n}{4}\ ,\frac{n}{2}\right] \\
 & {}_0A_0^{+}+{}_{\pi}A_0^{+}+{}_{\pi}A_0^{-} & k=\frac{\pi}{2}\ ,\ \ m=0\ ,\frac{n}{2} \\
 & {}_0A_0^{+}+{}_{\pi}A_{n/2}^{+}+{}_{\pi}A_{n/2}^{-} & k=\frac{\pi}{2}\ ,\ \ m=\pm\frac{n}{4} \\
[{}_0E_m^{-m\,2}]=[{}_{\pi}E_m^{-m\,2}]= & {}_0A_0^{+}+{}_0E_{2m}^{-2m} & k=\frac{\pi}{2}\ ,\ \ m\in\left[0,\frac{n}{4}\right] \\
 & {}_0A_0^{+}+{}_0E_{-2m+n}^{2m-n} & k=\frac{\pi}{2}\ ,\ \ m\in\left[\frac{n}{4}\ ,\frac{n}{2}\right] \\
 & {}_0A_0^{+}+{}_0A_{n/2}^{+}+{}_0A_{n/2}^{-} & k=\frac{\pi}{2}\ ,\ \ m=\pm\frac{n}{4}\ .
\end{array}
$$

The reduction of the polar- and axial-vector representations gives

$$ V=A=\begin{cases} {}_0A_0^{-}+{}_{\kappa}^{-\kappa}E_0^{0} & n=1\ , \\ {}_0A_0^{-}+{}_{\kappa}^{-\kappa}E_1^{1} & n=2\ , \\ {}_0A_0^{-}+{}_{\kappa}^{-\kappa}E_1^{-1} & n>2\ , \end{cases} $$

with κ given in (A1). z components of the translations and rotations transform according to the ${}_0A_0^{-}$, while the other representations correspond to the standard combinations of the x and y components.

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