Translation Groups; Introduction to Bands and Reciprocal Space©

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The One-dimensional Translation Group

If chemists wish to understand the symmetry properties of a particular molecule's vibrational modes, they know that they must understand the transformation properties of the irreducible representations of that molecule's point group. Likewise, chemists are familiar with the use of point groups to simplify and/or classify molecular orbitals. Without an entirely analogous accounting for symmetry, the problem of understanding the "molecular" orbitals of an infinite chain system such as the crystalline *trans*-polyacetylene depicted below would seem to be intractable. However, all crystals

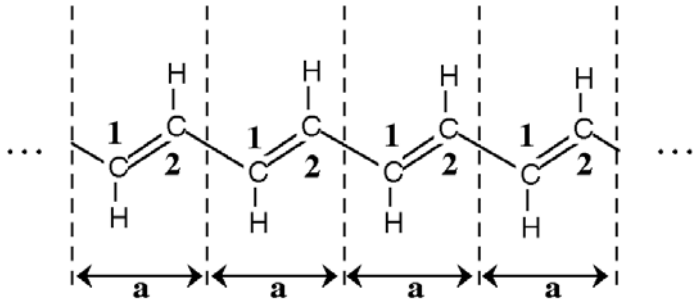
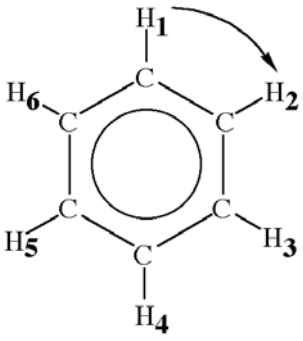


Figure 1. The chain structure of *trans*-polyacetylene.

have a tremendous amount of *translational* symmetry and *trans*-polyacetylene is just a one-dimensional example.

When we imagine the application of a point group symmetry operation to a molecule, we think of the all atoms of the molecule as being carried to the position that an equivalent atom had previously occupied. A six-fold rotation applied to benzene carries H_1 to the position occupied by H_2, H_2 to the position occupied by H_3, and so on.



A translation operation, **t**, when applied to the one-dimensional chain, simply moves the contents of a given unit

cell into the neighboring cell. If the translation operation is applied twice in succession ($\mathbf{t}^2$), the all the atoms of the chain are shifted by two unit cell lengths, and so on ... for the operations $\mathbf{t}^3$, $\mathbf{t}^4$….

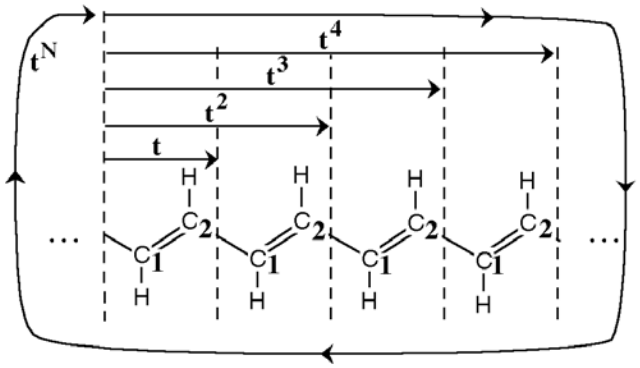


Figure 2. The translations of the $\mathbf{T_N}$ group for a polyacetylene chain.

The *group* of translation operators (which we shall call $\mathbf{T_N}$) is quite analogous to a pure rotation group, $\mathbf{C_N}$. In fact, if we impose one artificial constraint on the translation group, its structure will be exactly like the rotation group. Up to this point we have ignored the question of what happens to the *ends* of a chain when we apply a translation operation, an attitude which would be justified if the chain had infinite length. Rather than assuming the chain is infinite, we will instead assume that an infinite chain is well approximated as a *ring* with a very large radius of curvature. We assume that if we had a ring with $\mathbf{C_N}$ symmetry it would be physically indistinguishable from an infinite chain (or at least a chain with N unit cells) as long as N is very large. Obviously, this is not a reasonable assumption if we are interested in atoms that are at or near the end of the chain, but it is quite reasonable if we are interested in the properties of the chain that are determined by the bulk of the atoms which are far removed from the ends (on the molecular scale). To state our assumption mathematically, we assume that if we apply the translation operation N times ($\mathbf{t}^N$), then we simply return the contents of each unit cell to their original position (i.e.., $\mathbf{t}^N = E$ — the identity operation). Naturally, this is the same result we obtain when we apply a $\mathbf{C}^N$ operation to a N-membered ring system.

All the properties of a $\mathbf{C_N}$ group are shared by the *isomorphic* $\mathbf{T_N}$ group. The multiplication table for the $\mathbf{C_N}$ group looks just like the multiplication table for the $\mathbf{T_N}$ group, only the labels of the symmetry operations change. In the rotation group, all the operations commute with one another: $\mathbf{C}^m\mathbf{C}^n = \mathbf{C}^n\mathbf{C}^m$; likewise for the translation group: $\mathbf{t}^m\mathbf{t}^n = \mathbf{t}^n\mathbf{t}^m$. Both $\mathbf{C_N}$ and $\mathbf{T_N}$ are *cyclic, abelian* groups. As a result, each of the translation operators ($\mathbf{t}^m$) is in its own *class*. There are *N* distinct one-dimensional irreducible representations for the group $\mathbf{T_N}$, just as for $\mathbf{C_N}$. $\mathbf{T_N}$ and $\mathbf{C_N}$ have identical character tables (as any pair of isomorphic groups must; compare, for example, the multiplication tables and character tables for the isomorphic groups C_{3v} and D_3). As far as group theory is concerned, we can handle chain systems with machinery that is no different than for point groups. However, we need to introduce the notation that is used for crystals.

Let us take a look at the structure of a character table for the translation group $\mathbf{T_N}$ for a one-dimensional system$\left(\varepsilon = e^{2\pi i/N}\right)$, written in a way directly comparable to presentation given by Cotton (p. 96, 3rd edition):

	$\mathbf{t}$	$\mathbf{t^2}$	$\mathbf{t^3}$	$\cdots$	$\mathbf{t^{N-1}}$	$\mathbf{t^N} = E$
Γ^1	ε	ε^2	ε^3	$\cdots$	ε^{N-1}	ε^N
Γ^2	ε^2	ε^4	ε^6	$\cdots$	ε^{2N-2}	ε^{2N}
Γ^3	ε^3	ε^6	ε^9	$\cdots$	ε^{3N-3}	ε^{3N}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
Γ^{N-1}	ε^{N-1}	ε^{2N-2}	ε^{3N-3}	$\cdots$	$\varepsilon^{(N-1)^2}$	$\varepsilon^{N(N-1)}$
Γ^N	ε^N	ε^{2N}	ε^{3N}	$\cdots$	$\varepsilon^{N(N-1)}$	ε^{N^2}

Table 1. Character table for the $\mathbf{T_N}$ group.

We recognize that $\varepsilon^N = \left(e^{2\pi i/N}\right)^N = e^{2\pi i} = 1$, so that the above table can be simplified to read as indicated in Table 2 (just as done for the $\mathbf{C_5}$ group on p. 97 of Cotton).

	$\mathbf{t}$	$\mathbf{t^2}$	$\mathbf{t^3}$	$\cdots$	$\mathbf{t^{N-1}}$	$\mathbf{t^N} = E$
Γ^1	ε	ε^2	ε^3	$\cdots$	ε^{N-1}	1
Γ^2	ε^2	ε^4	ε^6	$\cdots$	ε^{2N-2}	1
Γ^3	ε^3	ε^6	ε^9	$\cdots$	ε^{3N-3}	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
Γ^{N-1}	ε^{N-1}	ε^{2N-2}	ε^{3N-3}	$\cdots$	$\varepsilon^{(N-1)^2}$	1
Γ^N	1	1	1	$\cdots$	1	1

Table 2. A rewritten character table for the $\mathbf{T_N}$ group.

Now let us complicate matters and introduce many redundant irreducible representations to top of this table, that we will label as Γ^0, Γ^{-1}, Γ^{-2}, etc…. We will furthermore add additional redundant representations to the bottom of the table that we will label as Γ^{N+1}, Γ^{N+2}, etc…. Because of the nature of the complex number ε, we see that Γ^0 is equivalent to Γ^N, Γ^{-1} is equivalent to Γ^{N-1}, Γ^{N+1} is equivalent to Γ^1, Γ^{N+2} is equivalent to Γ^2, and so on. We then have an "extended" character table in which all Γ^{mN+j} (m and j are integers) are identical with Γ^j.

	$\mathbf{t}$	$\mathbf{t^2}$	$\mathbf{t^3}$	$\cdots$	$\mathbf{t^{N-1}}$	$\mathbf{t^N} = E$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\cdots$	$\vdots$	$\vdots$
Γ^{-2}	ε^{-2}	ε^{-4}	ε^{-6}	$\cdots$	ε^{-2N+2}	1
Γ^{-1}	ε^{-1}	ε^{-2}	ε^{-3}	$\cdots$	$\varepsilon^{-(N-1)}$	1
Γ^0	$\varepsilon^0 = 1$	1	1	$\cdots$	1	1
Γ^1	ε^1	ε^2	ε^3	$\cdots$	ε^{N-1}	1
Γ^2	ε^2	ε^4	ε^6	$\cdots$	ε^{2N-2}	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
Γ^{N-1}	ε^{N-1}	ε^{2N-2}	ε^{3N-3}	$\cdots$	$\varepsilon^{(N-1)^2}$	1
Γ^N	1	1	1	$\cdots$	1	1
Γ^{N+1}	$\varepsilon^{N+1} = \varepsilon$	ε^2	ε^3	$\cdots$	ε^{N-1}	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 3. Character table for the $\mathbf{T_N}$ group, including redundant representations outside the dashed lines.

Because of the redundancies and periodicity that relates rows of the above table we can choose any set of adjacent N rows in the table and have a complete set of irreducible representations for the translational group $\mathbf{T_N}$. In particular, we can choose

the set of N representations that extend from $\Gamma^{-N/2+1}$ to $\Gamma^{N/2}$ (Assume, for the sake of convenience, that N is an even number. No serious complications arise if N is odd.) Further, we replace factors of ε^N, ε^{2N}, ε^{3N},… by 1 and $\varepsilon^{N/2}$, $\varepsilon^{3N/2}$, $\varepsilon^{5N/2}$,… by -1. Then our character table takes the appearance we see below:

	$\mathbf{t}$	$\mathbf{t^2}$	$\mathbf{t^3}$	$\cdots$	$\mathbf{t^{N-1}}$	$\mathbf{t^N} = E$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\cdots$	$\vdots$	$\vdots$
$\Gamma^{-N/2}$	-1	1	-1	$\cdots$	-1	1
$\Gamma^{-N/2+1}$	$-\varepsilon$	ε^2	$-\varepsilon^3$	$\cdots$	$-\varepsilon^{-1}$	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\cdots$	$\vdots$	$\vdots$
Γ^{-1}	ε^{-1}	ε^{-2}	ε^{-3}	$\cdots$	$\varepsilon^{-(N-1)}$	1
Γ^0	1	1	1	$\cdots$	1	1
Γ^1	ε^1	ε^2	ε^3	$\cdots$	ε^{N-1}	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\cdots$	$\vdots$	$\vdots$
$\Gamma^{N/2}$	-1	1	-1	$\cdots$	-1	1
$\Gamma^{N/2+1}$	$-\varepsilon$	ε^2	$-\varepsilon^3$	$\cdots$	$-\varepsilon^{-1}$	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 4. $\mathbf{T_N}$: nonredundant representations are included between dashed lines.

where we have intermittently used the relations $\varepsilon^N = 1$ and $\varepsilon^{mN+j} = \varepsilon^j$ for integral m. In handling the symmetry of one-dimensional chain systems, this set of irreducible representations is the usual choice.

The reader should recognize that we have done nothing in the above but rearrange the character table for the cyclic group $\mathbf{T_N}$. The basic group theory for the cyclic, abelian $\mathbf{T_N}$ group is indistinguishable from that for a $\mathbf{C_N}$ rotation group and all the properties of the $\mathbf{C_N}$ group are naturally the same for $\mathbf{T_N}$. We are now in a position to make some changes in notation that will allow us to make direct connections to the language of solid state scientists in dealing with systems with translational symmetry (crystals!).

As we indicated in the opening remarks, the translation group is used for handling systems that are very large (effectively "infinite") on the molecular scale. For example, if we are concerned with the electronic structure of polyacetylene, we can safely assume that a treatment suitable for describing the bulk electronic properties of an "infinite" polymer would virtually as good for a finite polymer with 40,000 unit cells as it would for a polymer with 60,000 unit cells. Because we are interested in the limit where polymers are very long, we want to somehow eliminate the N dependence that remains in our discussion of the translation group.

The N dependence of the translation group is customarily eliminated (or at least hidden) by introducing a variable, k ,that is simply proportional to the labels for the irreducible representations:

$$k = \left(\frac{1}{a}\right) \cdot \left(\frac{j}{N}\right); \qquad -\frac{1}{2a} < k \le \frac{1}{2a}.$$

where the range of k is determined by the fact that in the list of unique irreducible representations, j runs from $-(N/2)+1$ to $(N/2)$. Any function that "belongs" to given irreducible representation Γ^j is now said to "belong" to a given k. With the above, we note that $\varepsilon^j = \mathrm{e}^{2\pi i k a}$ so that the characters for any of the N irreducible representations can be written in the same form,

	$\mathbf{t}$	$\mathbf{t^2}$	$\mathbf{t^3}$	$\cdots$	$\mathbf{t^{N-1}}$	$\mathbf{t^N} = E$
$\Gamma(k)$	$e^{2\pi i(k\bullet a)}$	$e^{2\pi i(k\bullet 2a)}$	$e^{2\pi i(k\bullet 3a)}$	$\cdots$	$e^{-2\pi i(k\bullet a)}$	1

We must remember that k takes on exactly N discrete values within the range $-1/(2a) < k \le 1/(2a)$. We should note that our definition for k is not universal; it is common in physics texts to define $k = (2\pi/a)(j/N)$; $-(\pi/a) < k \le (\pi/a)$, which eliminates the factors of 2π that explicitly appear in the characters but which are instead included in the definition of k. The usefulness of this form of the translation group representations will become more apparent in later sections.