# E

# Group Theory Aspects of Carbon Nanotubes

In this appendix we provide information needed for solving problems related to carbon nanotubes (see Sect. 9.4). Carbon nanotubes in general exhibit compound rotation-translation operations and therefore belong to nonsymmorphic space groups. From the symmetry point of view, there are two types of carbon nanotubes, namely chiral and achiral tubes. We here discuss the structure of carbon nanotubes and provide the character tables for the group of the wavevectors at $k = 0$ and $k \neq 0$, for both chiral and achiral tubes [8].

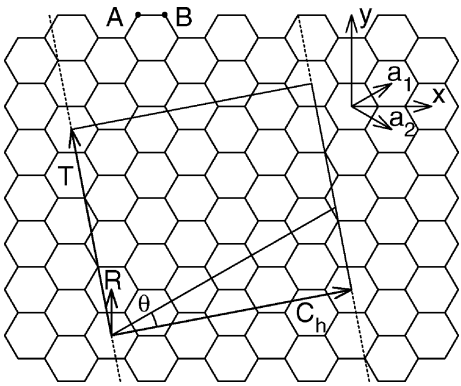


**Fig. E.1.** An unrolled carbon nanotube projected on a graphene layer (a single layer of crystalline graphite). When the nanotube is rolled up, the chiral vector $\boldsymbol{C}_h$ turns into the circumference of the cylinder, and the translation vector $\boldsymbol{T}$ is aligned along the cylinder axis. $\boldsymbol{R}$ is the symmetry vector (Sect. E.4) and $\theta$ is the chiral angle. The unit vectors $(\boldsymbol{a}_1, \boldsymbol{a}_2)$ of the graphene layer are indicated in the figure along with the inequivalent A and B sites within the unit cell of the graphene layer [64]

## E.1 Nanotube Geometry and the $(n, m)$ Indices

A single wall carbon nanotube (SWNT) is constructed starting from a graphene layer (see Fig. E.1) by rolling it up into a seamless cylinder. The nanotube structure is uniquely determined by the chiral vector $\boldsymbol{C}_h$ which spans the circumference of the cylinder when the graphene layer is rolled up into a tube. The chiral vector can be written in the form

$$\boldsymbol{C}_h = n\boldsymbol{a}_1 + m\boldsymbol{a}_2\,, \tag{E.1}$$

where the vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ bounding the unit cell of the graphene layer contain two distinct carbon atom sites $A$ and $B$, as shown in Fig. E.1, while $n$ and $m$ are arbitrary integer numbers. In the shortened $(n, m)$ form, the chiral vector is written as a pair of integers. The $(n, m)$ notation is widely used to characterize the geometry of each distinct $(n, m)$ nanotube [63, 64].

The nanotube can also be characterized by its diameter $d_t$ and chiral angle $\theta$, which determine the length $C_h = |\boldsymbol{C}_h| = \pi d_t$ of the chiral vector and its orientation on the graphene layer (see Fig. E.1). Both $d_t$ and $\theta$ are expressed in terms of the indices $n$ and $m$ by the relations $d_t = a\sqrt{n^2 + nm + m^2}/\pi$ and $\tan\theta = \sqrt{3}m/(2n+m)$, as one can derive from Fig. E.1, where $a = \sqrt{3}a_{\mathrm{C-C}} = 0.246\,\mathrm{nm}$ is the lattice constant for the graphene layer and $a_{\mathrm{C-C}} = 0.142\,\mathrm{nm}$ is the nearest neighbor C–C distance. As an example, the chiral vector $\boldsymbol{C}_h$ shown in Fig. E.1 is given by $\boldsymbol{C}_h = 4\boldsymbol{a}_1 + 2\boldsymbol{a}_2$, and thus the corresponding nanotube can be identified by the integer pair $(4, 2)$. Due to the sixfold symmetry of the graphene layer, all nonequivalent nanotubes can be characterized by the $(n, m)$ pairs of integers where $0 \le m \le n$. It is also possible to define nanotubes with opposite handedness, for which $0 \le n \le m$ [65]. The nanotubes are classified as chiral $(0 < m < n)$ and achiral ($m = 0$ or $m = n$), which in turn are known as zigzag ($m = 0$) and armchair ($m = n$) nanotubes (see Figs. 9.11 and E.1).

## E.2 Lattice Vectors in Real Space

To specify the symmetry properties of carbon nanotubes as 1D systems, it is necessary to define the lattice vector or translation vector $\boldsymbol{T}$ along the nanotube axis and normal to the chiral vector $\boldsymbol{C}_h$ defined in Fig. E.1. The vectors $\boldsymbol{T}$ and $\boldsymbol{C}_h$ define the unit cell of the 1D nanotube. The translation vector $\boldsymbol{T}$, of a general chiral nanotube as a function of $n$ and $m$, can be written as

$$\boldsymbol{T} = (t_1\boldsymbol{a_1} + t_2\boldsymbol{a_2}) = [(2m+n)\boldsymbol{a}_1 - (2n+m)\boldsymbol{a}_2]/d_R\,, \tag{E.2}$$

with a length $T = \sqrt{3}C_h/d_R$, where $d$ is the greatest common divisor of $(n, m)$, and $d_R$ is the greatest common divisor of $2n + m$ and $2m + n$. Then $d$ and $d_R$ are related by

$$d_R = \begin{cases} d & \text{if } n-m \text{ is not a multiple of } 3d \\ 3d & \text{if } n-m \text{ is a multiple of } 3d\,. \end{cases} \tag{E.3}$$

For the $(4,2)$ nanotube shown in Fig. E.1, we have $d_R = d = 2$ and $(t_1, t_2) = (4, -5)$. For armchair and zigzag achiral tubes, $T = a$ and $T = \sqrt{3}a$, respectively. The unit cell of an unrolled nanotube on a graphene layer is a rectangle bounded by the vectors $\boldsymbol{C}_h$ and $\boldsymbol{T}$ (see the rectangle shown in Fig. E.1 for the $(4,2)$ nanotube). The area of the nanotube unit cell can be easily calculated as a vector product of these two vectors, $|\boldsymbol{C}_h \times \boldsymbol{T}| = \sqrt{3}a^2(n^2+nm+m^2)/d_R$. Dividing this product by the area of the unit cell of a graphene layer $|\boldsymbol{a}_1 \times \boldsymbol{a}_2| = \sqrt{3}a^2/2$, one can get the number of hexagons in the unit cell of a nanotube,

$$N = \frac{2(n^2+nm+m^2)}{d_R}\,. \tag{E.4}$$

For the $(4,2)$ nanotube we have $N = 28$, so that the unit cell of the $(4,2)$ nanotube (see the rectangle shown in Fig. E.1) contains 28 hexagons, or $2\times 28 = 56$ carbon atoms. For armchair $(n,n)$ and zigzag $(n,0)$ nanotubes, $N = 2n$.

## E.3 Lattice Vectors in Reciprocal Space

The unit cell of a graphene layer is defined by the vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$. The graphene reciprocal lattice unit vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ can be constructed from $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ using the standard definition $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$, where $\delta_{ij}$ is the Kroneker delta symbol. In Fig. E.2, we show a diagram for the real space unit cell of a graphene sheet (Fig. E.2(a)) and its corresponding reciprocal lattice unit cell

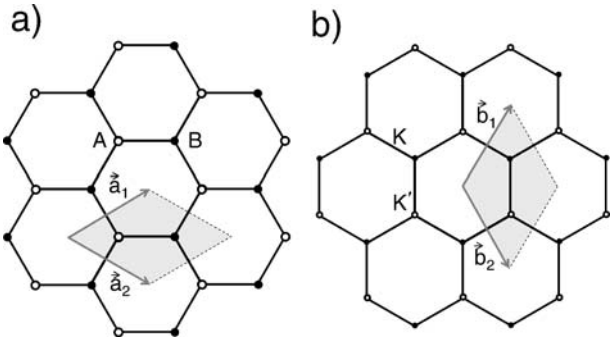


**Fig. E.2.** (**a**) Real space structure of a graphene layer. The gray rhombus represents the graphene unit cell with the lattice vectors denoted by $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ delimiting it. Note that this area encloses a total of two atoms, one A atom and one B atom. (**b**) Reciprocal space unit cell of the graphene layer denoted by the unit vectors $\boldsymbol{b_1}$ and $\boldsymbol{b_2}$. Note also that the reciprocal space structure has two inequivalent points $K$ and $K'$ [8]

is shown in Fig. E.2(b). Note the rotation by the angle 30° of the hexagons in real space (Fig. E.2(a)) with respect to those in reciprocal space (Fig. E.2(b)).

In a similar fashion, the reciprocal space of a nanotube can be constructed, if we consider the nanotube as a 1D system with an internal structure that is composed of the $2N$ atoms in its unit cell and with a translational symmetry given by the translation vector $\boldsymbol{T}$. The reciprocal space of the nanotube can be constructed by finding a pair of reciprocal lattice vectors $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ which satisfy: $\boldsymbol{C}_h \cdot \boldsymbol{K}_1 = \boldsymbol{T} \cdot \boldsymbol{K}_2 = 2\pi$ and $\boldsymbol{C}_h \cdot \boldsymbol{K}_2 = \boldsymbol{T} \cdot \boldsymbol{K}_1 = 0$. Due to the spatial confinement of the nanotube in the radial direction, the vector $\boldsymbol{C}_h$ does not play the role of a translation vector but rather of a generator of pure rotations, and the relation $\boldsymbol{C}_h \cdot \boldsymbol{K}_1 = 2\pi$ can only be satisfied for integer multiples of $2\pi/d_t$, where $d_t$ is the diameter of the nanotube.

## E.4 Compound Operations and Tube Helicity

All multiples of the translation vector $\boldsymbol{T}$ will be translational symmetry operations of the nanotube [73]. However, to be more general, it is necessary to consider that any lattice vector

$$\boldsymbol{t}_{p,q} = p\boldsymbol{a}_1 + q\boldsymbol{a}_2\,, \tag{E.5}$$

with $p$ and $q$ integers, of the unfolded graphene layer will also be a symmetry operation of the tube. In fact, the symmetry operation that arises from $\boldsymbol{t}_{p,q}$ will appear as a screw translation of the nanotube. Screw translations are combinations of a rotation ($R_\phi$) by an angle $\phi$ and a small translation of $\boldsymbol{\tau}$ in the axial direction of the nanotube, and can be written as $\{R_\phi|\tau\}$, using the notation common for space group operations [8, 64].

Any lattice vector $\boldsymbol{t}_{p,q}$ can also be written in terms of components of the nanotube lattice vectors, $\boldsymbol{T}$ and $\boldsymbol{C}_h$, as

$$\boldsymbol{t}_{p,q} = \boldsymbol{t}_{u,v} = (u/N)\boldsymbol{C}_h + (v/N)\boldsymbol{T}\,, \tag{E.6}$$

where $u$ and $v$ are negative or positive integers given by

$$u = \frac{(2n+m)p + (2m+n)q}{d_R} \tag{E.7}$$

and

$$v = mp - nq\,. \tag{E.8}$$

The screw translation of the nanotube which is associated with the graphene lattice vector $\boldsymbol{t}_{u,v}$ can then be written as

$$\boldsymbol{t}_{u,v} = \{C_N^u|vT/N\}\,, \tag{E.9}$$

where $C_N^u$ is a rotation of $u(2\pi/N)$ around the nanotube axis, and $\{E|vT/N\}$ is a translation of $vT/N$ along the nanotube axis, with $T$ being the magnitude

of the primitive translation vector $\boldsymbol{T}$, and $E$ being the identity operation. It is clear that if a screw vector $\{C_N^u|vT/N\}$ is a symmetry operation of the nanotube, then the vectors $\{C_N^u|vT/N\}^s$, for any integer value of $s$, are also symmetry operations of the nanotube. The number of hexagons in the unit-cell $N$ assumes the role of the "order" of the screw axis, since the symmetry operation $\{C_N^u|vT/N\}^N = \{E|vT\}$, where $E$ is the identity operator, and $v\boldsymbol{T}$ is a primitive translation of the nanotube.

The nanotube structure can be obtained from a small number of atoms by using any choice of two noncolinear screw vectors $\{C_N^{u_1}|v_1T/N\}$ and $\{C_N^{u_2}|v_2T/N\}$. The two vectors will be colinear if there exists a pair of integers $s$ and $l$ different from 1, for which $lu_1 = su_2 + \lambda N$, and $lv_1 = sv_2 + \gamma T$, where, $\lambda$ and $\gamma$ are two arbitrary integers. The area of the nanotube cylindrical surface delimited by these two noncolinear vectors can be regarded as a reduced unit cell. Note that the number of atoms in this reduced unit cell is given by the ratio between the area delimited by these vectors ($|\boldsymbol{t}_{u_1,v_1} \times \boldsymbol{t}_{u_2,v_2}|$) and the area of the unit cell of a graphene sheet ($|\boldsymbol{a}_1 \times \boldsymbol{a}_2|$) multiplied by 2, which is the number of carbon atoms in the graphene unit cell. Thus the number of atoms in the reduced unit cell defined by $t_{u_1,v_1}$ and $t_{u_2,v_2}$ is given by

$$2\frac{|\boldsymbol{t}_{u_1,v_1} \times \boldsymbol{t}_{u_2,v_2}|}{|\boldsymbol{a}_1 \times \boldsymbol{a}_2|} = 2\frac{|v_2u_1 - u_2v_1|}{N}\,. \tag{E.10}$$

It is important to point out that, in this case, the nanotube ceases to be described as a quasi-1D system, but as a system with two quasitranslational dimensions, which are generated by the two screw vectors.

There are many combinations of screw vectors which can be used to construct the structure of the nanotube. These combinations can be divided into four categories: helical–helical, linear–helical, helical–angular, and linear–angular, as described below. Either one of these constructions can be used to obtain the nanotube structure. The helical–helical construction is characterized by choosing two general screw vectors, for the construction of the nanotube structure (see Fig. E.3(a)). Although this scheme permits the definition of a 2-atom unit cell, the unit cell does not exhibit the full symmetries of the nanotube, and thus is inadequate for representing the nanotube. The linear–helical scheme is characterized by using the translation vector $\boldsymbol{T}$ and a general screw vector as unit vectors (see Fig. E.3(b)). This scheme maintains the translational symmetry of the nanotube, but not the point group operations, and it also permits the definition of a two-atom unit cell. In the helical–angular construction, a general screw vector is used along with a vector in the circumferential direction of the nanotube (see Fig. E.3(c)). This construction also permits the definition of a 2-atom unit cell. However, the 2-atom unit cell does not exhibit many of the symmetries of the nanotube. Instead it is convenient to define a $2d$-atom unit cell, where the integer $d$ is given by $d = gcd(n, m)$, and this unit cell will exhibit all the point group symmetry operations of the nanotube, but not the translational symmetry. The linear–angular construction uses as unit vectors the translational vector

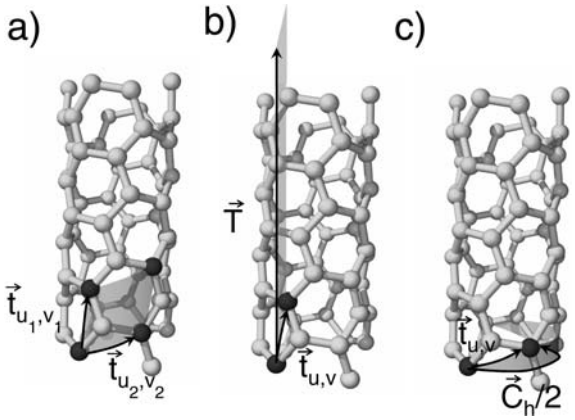


**Fig. E.3.** The 2-atom reduced unit cell for the: (**a**) helical–helical, (**b**) linear–helical, and (**c**) helical–angular construction for a $(4, 2)$ nanotube. In (**b**) the deformed rhombus, which delimits the reduced unit cell that connects points both inside and outside the nanotube unit cell, had to be truncated to stay within the figure [8]

$\boldsymbol{T}$ and a vector in the circumferential direction, and thus parallel to $\boldsymbol{C}_h$. The linear–angular construction does not permit the definition of a 2-atom unit cell. However, by choosing the vector in the circumferential direction to be $\boldsymbol{C}_h$, the total unit cell of the nanotube, which exhibits all the translational and point symmetries of the nanotube, is restored.

## E.5 Character Tables for Carbon Nanotubes

In this section we present the character tables for dealing with carbon nanotubes. Tables E.1 and E.2 give the character tables for the group of the wavevectors for chiral carbon nanotubes, at $k = 0, \pi/T$ and $0 < k < \pi/T$, respectively. Tables E.3 and E.4 give the character tables for the group of the wavevectors for achiral carbon nanotubes, at $k = 0, \pi/T$ and $0 < k < \pi/T$, respectively. Some of the point symmetry operations in these tables are shown in Fig. E.4.

**Table E.1.** Character table for the group of the wavevectors $k = 0$ and $k = \pi/T$ for chiral tubes

| $D_N$ | $\{E\|0\}$ | $2\{C_N^u\|vT/N\}$ | $2\{C_N^u\|vT/N\}^2$ | ... | $2\{C_N^u\|vT/N\}^{(N/2)-1}$ | $2\{C_N^u\|vT/N\}^{N/2}$ | $(N/2)\{C_2'\|0\}$ | $(N/2)\{C_2''\|0\}$ |
|---|---|---|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | ... | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | 1 | ... | 1 | 1 | $-1$ | $-1$ |
| $B_1$ | 1 | $-1$ | 1 | ... | $(-1)^{(N/2-1)}$ | $(-1)^{N/2}$ | 1 | $-1$ |
| $B_2$ | 1 | $-1$ | 1 | ... | $(-1)^{(N/2-1)}$ | $(-1)^{N/2}$ | $-1$ | 1 |
| $E_1$ | 2 | $2\cos 2\pi/N$ | $2\cos 4\pi/N$ | ... | $2\cos 2(N/2-1)\pi/N$ | $-2$ | 0 | 0 |
| $E_2$ | 2 | $2\cos 4\pi/N$ | $2\cos 8\pi/N$ | ... | $2\cos 4(N/2-1)\pi/N$ | 2 | 0 | 0 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $E_{(N/2-1)}$ | 2 | $2\cos 2(N/2-1)\pi/N$ | $2\cos 4(N/2-1)\pi/N$ | ... | $2\cos 2(N/2-1)^2\pi/N$ | $2\cos(N/2-1)\pi$ | 0 | 0 |

This group is isomorphic to the point group $D_N$

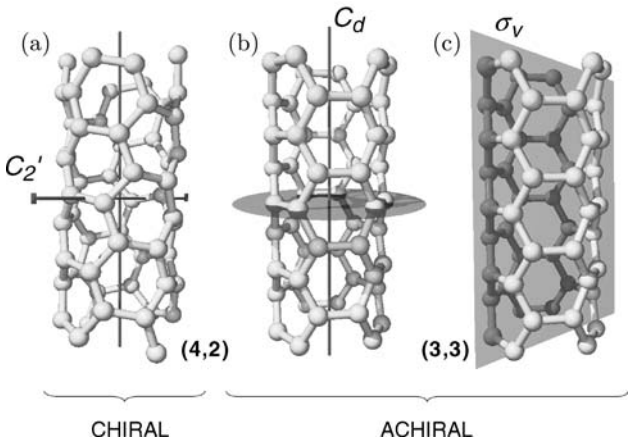


**Fig. E.4.** (**a**) Unit cell of the chiral (4,2) nanotube, showing the $C_d$ rotation around the nanotube axis, with $d = 2$, and one of the $C_2'$ rotations perpendicular to the nanotube axis. A different class of two-fold rotations ($C_2''$), which is present for both chiral and achiral nanotubes, is not shown here. (**b**) A section of an achiral armchair (3,3) nanotube is shown emphasizing the horizontal mirror plane $\sigma_h$ and the symmetry operation $C_d$, with $d = 3$. (**c**) The same (3,3) armchair nanotube is shown but now emphasizing of the vertical mirror planes $\sigma_v$ [8]

**Table E.2.** Character table for the group of the wavevector $0 < k < \pi/T$ for chiral nanotubes

| $C_N$ | $\{E\|0\}$ | $\{C_N^u\|vT/N\}^1$ | $\{C_N^u\|vT/N\}^2$ | $\cdots$ | $\{C_N^u\|vT/N\}^\ell$ | $\cdots$ | $\{C_N^u\|vT/N\}^{N-1}$ |
|---|---|---|---|---|---|---|---|
| $A$ | 1 | 1 | 1 | $\cdots$ | 1 | $\cdots$ | 1 |
| $B$ | 1 | –1 | 1 | $\cdots$ | $(-1)^\ell$ | $\cdots$ | –1 |
| $E_{\pm1}$ | $\left\{\begin{matrix}1\\1\end{matrix}\right.$ | $\begin{matrix}\epsilon\\\epsilon^*\end{matrix}$ | $\begin{matrix}\epsilon^2\\\epsilon^{*2}\end{matrix}$ | $\cdots$ | $\begin{matrix}\epsilon^\ell\\\epsilon^{*\ell}\end{matrix}$ | $\cdots$ | $\left.\begin{matrix}\epsilon^{N-1}\\\epsilon^{*(N-1)}\end{matrix}\right\}$ |
| $E_{\pm2}$ | $\left\{\begin{matrix}1\\1\end{matrix}\right.$ | $\begin{matrix}\epsilon^2\\\epsilon^{*2}\end{matrix}$ | $\begin{matrix}\epsilon^4\\\epsilon^{*4}\end{matrix}$ | $\cdots$ | $\begin{matrix}\epsilon^{2\ell}\\\epsilon^{*2\ell}\end{matrix}$ | $\cdots$ | $\left.\begin{matrix}\epsilon^{2(N-1)}\\\epsilon^{*2(N-1)}\end{matrix}\right\}$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $E_{\pm(\frac{N}{2}-1)}$ | $\left\{\begin{matrix}1\\1\end{matrix}\right.$ | $\begin{matrix}\epsilon^{\frac{N}{2}-1}\\\epsilon^{*\frac{N}{2}-1}\end{matrix}$ | $\begin{matrix}\epsilon^{2(\frac{N}{2}-1)}\\\epsilon^{*2(\frac{N}{2}-1)}\end{matrix}$ | $\cdots$ | $\begin{matrix}\epsilon^{\ell(\frac{N}{2}-1)}\\\epsilon^{*\ell(\frac{N}{2}-1)}\end{matrix}$ | $\cdots$ | $\left.\begin{matrix}\epsilon^{(N-1)(\frac{N}{2}-1)}\\\epsilon^{*(N-1)(\frac{N}{2}-1)}\end{matrix}\right\}$ |

This group is isomorphic to the point group $C_N$. The $\pm$ signs label the different representations with characters which are complex conjugates of each other. These irreducible representations are degenerate due to time reversal symmetry. The complex number $\epsilon$ is $e^{2\pi i/N}$.

**Table E.3.** Character table for the group of the wavevectors $k = 0$ and $k = \pi/T$ for achiral carbon tubes. This group is isomorphic to the point group $D_{2nh}$

| $D_{2nh}$ | $\{E\|0\}$ | $\cdots$ | $2\{C_{2n}^u\|vT/2n\}^s$ | $\cdots$ | $\{C_{2n}^u\|vT/2n\}^n$ | $n\{C_2'\|0\}$ | $n\{C_2''\|0\}$ | $\{I\|0\}$ | $\cdots$ | $2\{IC_{2n}^u\|vT/2n\}^s$ | $\cdots$ | $\{\sigma_h\|0\}$ | $n\{\sigma_v'\|0\}$ | $n\{\sigma_v''\|T/2\}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $A_{1g}$ | 1 | $\cdots$ | 1 | $\cdots$ | 1 | 1 | 1 | 1 | $\cdots$ | 1 | $\cdots$ | 1 | 1 | 1 |
| $A_{2g}$ | 1 | $\cdots$ | 1 | $\cdots$ | 1 | –1 | –1 | 1 | $\cdots$ | 1 | $\cdots$ | 1 | –1 | –1 |
| $B_{1g}$ | 1 | $\cdots$ | $(-1)^s$ | $\cdots$ | $(-1)^n$ | –1 | 1 | 1 | $\cdots$ | $(-1)^s$ | $\cdots$ | $(-1)^n$ | –1 | 1 |
| $B_{2g}$ | 1 | $\cdots$ | $(-1)^s$ | $\cdots$ | $(-1)^n$ | 1 | –1 | 1 | $\cdots$ | $(-1)^s$ | $\cdots$ | $(-1)^n$ | 1 | –1 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | |
| $E_{\mu g}$ | 2 | $\cdots$ | $2\cos(\mu s\pi/n)$ | $\cdots$ | $2(-1)^\mu$ | 0 | 0 | 2 | $\cdots$ | $2\cos(\mu s\pi/n)$ | $\cdots$ | $2(-1)^\mu$ | 0 | 0 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $A_{1u}$ | 1 | $\cdots$ | 1 | $\cdots$ | 1 | 1 | 1 | –1 | $\cdots$ | –1 | $\cdots$ | –1 | –1 | –1 |
| $A_{2u}$ | 1 | $\cdots$ | 1 | $\cdots$ | 1 | –1 | –1 | –1 | $\cdots$ | –1 | $\cdots$ | –1 | 1 | 1 |
| $B_{1u}$ | 1 | $\cdots$ | $(-1)^s$ | $\cdots$ | $(-1)^n$ | –1 | 1 | –1 | $\cdots$ | $-(-1)^s$ | $\cdots$ | $(-1)^n$ | 1 | –1 |
| $B_{2u}$ | 1 | $\cdots$ | $(-1)^s$ | $\cdots$ | $(-1)^n$ | 1 | –1 | –1 | $\cdots$ | $-(-1)^s$ | $\cdots$ | $(-1)^n$ | –1 | 1 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | |
| $E_{\mu u}$ | 2 | $\cdots$ | $2\cos(\mu s\pi/n)$ | $\cdots$ | $2(-1)^\mu$ | 0 | 0 | –2 | $\cdots$ | $-2\cos(\mu s\pi/n)$ | $\cdots$ | $-2(-1)^\mu$ | 0 | 0 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |

The values of $s$ and $\mu$ span the integer values between 1 and $n - 1$.

**Table E.4.** Character table for the group of the wavevectors $0 < k\pi/T$ for achiral carbon nanotubes

| $C_{2nv}$ | $\{E\|0\}$ | $2\{C_{2n}^u\|vT/2n\}^1$ | $\{C_{2n}^u\|vT/2n\}^2$ | ... | $2\{C_{2n}^u\|vT/2n\}^{n-1}$ | $\{C_{2n}^u\|vT/2n\}^n$ | $n\{\sigma_v'\|\tau'\}$ | $n\{\sigma_v''\|\tau''\}$ |
|---|---|---|---|---|---|---|---|---|
| $A'$ | 1 | 1 | 1 | ... | 1 | 1 | 1 | 1 |
| $A''$ | 1 | 1 | 1 | ... | 1 | 1 | −1 | −1 |
| $B'$ | 1 | −1 | 1 | ... | $(-1)^{(n-1)}$ | $(-1)^n$ | 1 | −1 |
| $B''$ | 1 | −1 | 1 | ... | $(-1)^{(n-1)}$ | $(-1)^n$ | −1 | 1 |
| $E_1$ | 2 | $2\cos\pi/n$ | $2\cos 2\pi/n$ | ... | $2\cos 2(n-1)\pi/n$ | −2 | 0 | 0 |
| $E_2$ | 2 | $2\cos 2\pi/n$ | $2\cos 4\pi/n$ | ... | $2\cos 4(n-1)\pi/n$ | 2 | 0 | 0 |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| $E_{(n-1)}$ | 2 | $2\cos(n-1)\pi/n$ | $2\cos 2(n-1)\pi/n$ | ... | $2\cos(n-1)^2\pi/n$ | $2\cos(n-1)\pi$ | 0 | 0 |

This group is isomorphic to the point group $C_{2nv}$. For zigzag nanotubes with $n$ odd, $\tau' = \tau'' = T/2$, while for armchair nanotubes and zigzag nanotubes with $n$ even, $\tau' = 0$ and $\tau'' = T/2$.