Toroidal molecules formed from three distinct carbon nanotubes

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Abstract In order to design nanotori for nanomechanical systems, perhaps involving oscillating components, precise physical parameters for the nanotori are necessary. Toroidal shaped molecules of carbon have been investigated previously by the present authors as constructed by connecting elbow sections formed from joining armchair and zigzag nanotubes through a pentagonal–heptagonal pair defect. In this paper, we extend this design by constructing the elbow structures from three distinct carbon nanotubes. Since for a toroidal molecule, there is a constraint on the bend angles in the elbow sections to add up to 360°, particular elbow types which can accommodate this requirement are (5,0)–(4,4)–(7,0) and (3,3)–(6,0)–(4,4). We adopt a least squares approach for the bond length to minimise the variation from the ideal carbon–carbon bond length, which is taken to be $\sigma = 1.42$ Å. Moreover, formulae for the mean generating radius of the nanotori and the mean radius of the nanotubes are obtained from certain integral expressions. This purely geometrical approach can be formally directly related to certain numerical energy minimisation methods used by a number of authors.

1 Introduction

Dunlap [1] first proposed the torus as a stable form of graphitic carbon. He constructs toroidal molecules by joining two different carbon nanotubes with matching radii and introduces the pentagon–heptagon pair [1–3]. Moreover, Dunlap [1–3] predicts

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that the molecule in all comprises 12 connecting sections occurring for the 360° turn and therefore, the tubule bend angle is 30° for each section. The energetic stability of molecules that are constructed based on the C_{60} fullerene and carbon nanotube structures are investigated by Itoh et al. [4], Ihara et al. [5] and Itoh and Ihara [6]. They find that these structures are more thermodynamically stable [5,7] and such toroidal shapes are expected to be physically more interesting than those of the two original structures [6]. Although, these theoretically proposed structures have not been confirmed by experiment [8], they are believed to give rise to fascinating electrical, magnetic and elastic properties arising from the pattern of the hexagonal rings [7].

In a recent paper Cox and Hill [9] show that certain toroidal molecules may be constructed from two types of carbon nanotubes, such that the bend angle and the two nanotubes lengths are determined by minimisation of the total squared deviations of the inter-atomic spacings from the ideal spacing $\sigma = 1.42$ Å. This procedure generates certain toroidal shaped molecules previously known to exist, along with numerous other toroidal molecular structures. The question arises as to the generality of the procedure, and whether or not we might determine other toroidal shaped molecules, such as ones constructed from three distinct nanotubes.

The major contribution of this paper is to examine the geometry of the basic repeatable units, comprising three distinct carbon nanotubes, which are needed to assemble the toroidal molecule. Subsequently and following [9], we join these repeating units according to the least squares minimisation of the deviations of the inter-atomic spacing from the ideal spacing $\sigma = 1.42$ Å. We comment that the least squares method can be related to the computer simulations for minimisation of the bonded interaction energy of covalent systems [10–13]. These authors assume that there are three main contributions to this bonded interatomic energy which arise from bond stretching, bond bend and bond torsion and which can be written as

$$E = \frac{1}{2}k_r(r - r_0)^2 + \frac{1}{2}k_\theta(\theta - \theta_0)^2 + \frac{1}{2}k_\tau(1 - \cos(n\phi - \phi_0)),$$

where k_r, k_θ and k_τ are certain bond stretching, bend angle and torsional constants, respectively, r_0, θ_0 and ϕ_0 are the equilibrium values of the bond length, bond angle and ideal phase for this bond type, respectively, and n is an integer. In terms of the force constants, k_r has the largest value [10–13] indicating that the bond stretching might be the dominant physical requirement for the bonded potential energy. Consequently, the purely geometrical approach adopted here corresponds to an energy approach where only the bond stretching energy is being taken into account.

We comment that in this paper, all the carbon nanotube sections are assumed to be either zigzag or armchair. This is because from previous studies only these two types of nanotubes are thought to form nanotori [1–3,14]. In addition, there is no experimental evidence to indicate that chiral tubes can be formed into toroidal structures [8]. The model formation for the elbow comprising three distinct carbon nanotubes is presented in the following section. In Sect. 3, the toroidal molecule constructed by connecting n sections of elbows is determined, and formulae for a mean radius of such tori and a mean radius of the tube are also given. The results and discussion are presented in Sect. 4. Finally, a summary is made in Sect. 5.

2 Model formation for elbow

In the present paper, we investigate the elbow structure required for toroidal molecules by joining three distinct carbon nanotubes of lengths $2\ell_1$, $2\ell_2$ and $2\ell_3$, and utilizing the least squares bond length method as proposed by Cox and Hill [9]. We note again that only zigzag and armchair carbon nanotubes are examined. The proposed model assumes that the basic repeating unit comprises tubes A and C as half unit lengths and tube B as one unit length. Further, it is assumed that the origin O of a rectangular Cartesian coordinate system (x, y, z) is located at the central point of tube B, such that the axis of tube B is aligned along the z-axis, as illustrated in Fig. 1.

We start by defining the ith terminal atom at a join location by position vectors $\mathbf{a}_i = (a_{ix}, a_{iy}, a_{iz})$, $\mathbf{b}_i = (b_{ix}, b_{iy}, b_{iz})$ and $\mathbf{c}_i = (c_{ix}, c_{iy}, c_{iz})$ for tubes A, B and C, respectively. At the junction of tubes A and B with x'-axis as shown in Fig. 2a, we perform a translation of the tube B in the negative z-direction by a length ℓ_{2A}, where we note that $2\ell_2 = \ell_{2A} + \ell_{2B}$ and ℓ_{2B} is as defined later in the text. Tube A is also translated
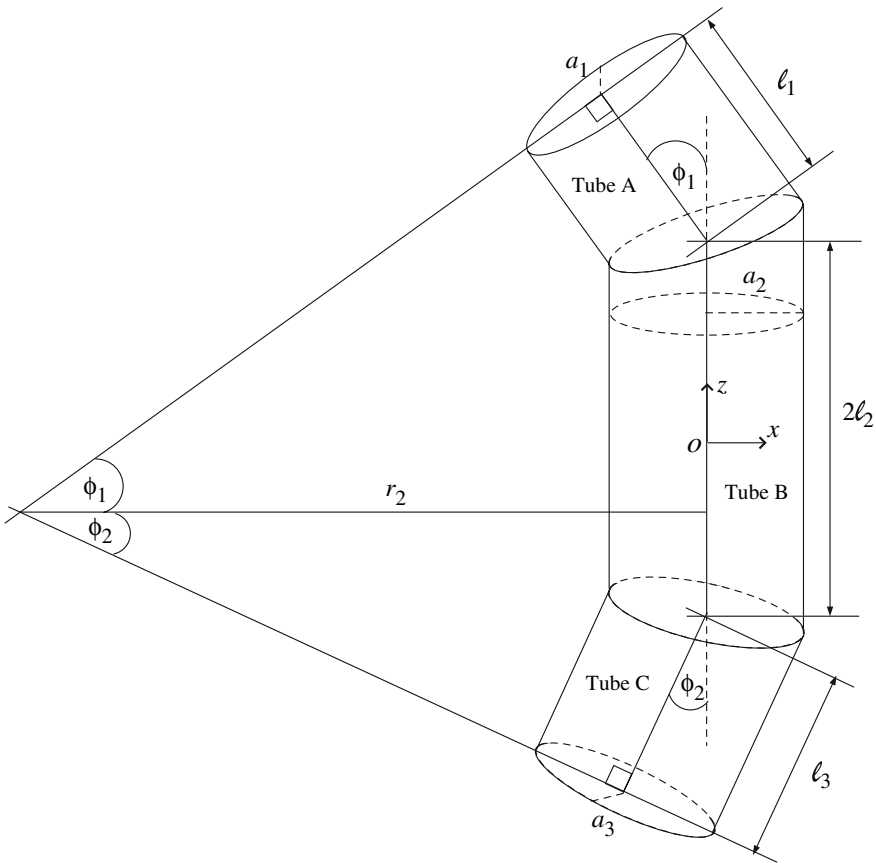
Fig. 1 Basic double elbow unit formed from three nanotube sections
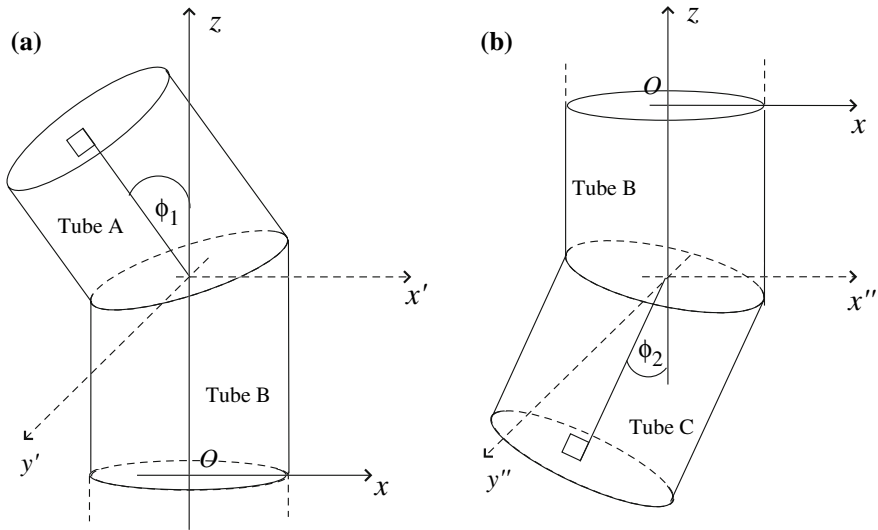
Fig. 2 Rectangular Cartesian coordinate system for two single nanotube elbows (a) for tubes A and B and (b) for tubes B and C

in the positive z-direction by a length ℓ_1 and rotated by an angle ϕ_1 about the y'-axis. Therefore, the Euclidean distance between the atoms at the junction is given by

$$|\mathbf{a}_i - \mathbf{b}_i| = \{[a_{ix}\cos\phi_1 + (a_{iz} + \ell_1)\sin\phi_1 - b_{ix}]^2 + (a_{iy} - b_{iy})^2$$
$$[(a_{iz} + \ell_1)\cos\phi_1 - a_{ix}\sin\phi_1 - (b_{iz} - \ell_{2A})]^2\}^{1/2}.$$

Similarly, at the junction of tubes B and C with x''-axis as shown in Fig. 2b, tube B is translated in the positive z-direction by a length ℓ_{2B}, tube C is translated in the negative z-direction by a length ℓ_3 and rotated by an angle ϕ_2 about the y''-axis. The distance between the atoms at the join location is then given by

$$|\mathbf{c}_i - \mathbf{b}_i| = \{[c_{ix}\cos\phi_2 + (c_{iz} - \ell_3)\sin\phi_2 - b_{ix}]^2 + (c_{iy} - b_{iy})^2$$
$$[(c_{iz} - \ell_3)\cos\phi_2 - c_{ix}\sin\phi_2 - (b_{iz} + \ell_{2B})]^2\}^{1/2}.$$

Given these distances between matching atoms, the procedure is to determine ℓ_1, ℓ_2, ℓ_3, ϕ_1 and ϕ_2 by minimising the least squares variation of these distances from the ideal carbon–carbon bond length which we take to be $\sigma = 1.42$ Å. Consequently, we are seeking to minimise the following objective functions,

$$f(\ell_1, \ell_{2A}, \phi_1) = \sum_i (|\mathbf{a}_i - \mathbf{b}_i| - \sigma)^2,$$
$$g(\ell_{2B}, \ell_3, \phi_2) = \sum_j (|\mathbf{c}_j - \mathbf{b}_j| - \sigma)^2.$$

(5,0)-(4,4)-(7,0)   (3,3)-(6,0)-(4,4)
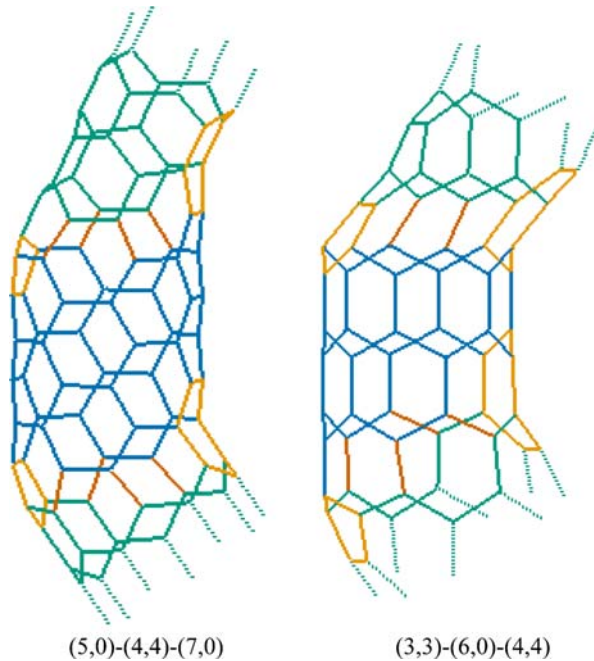
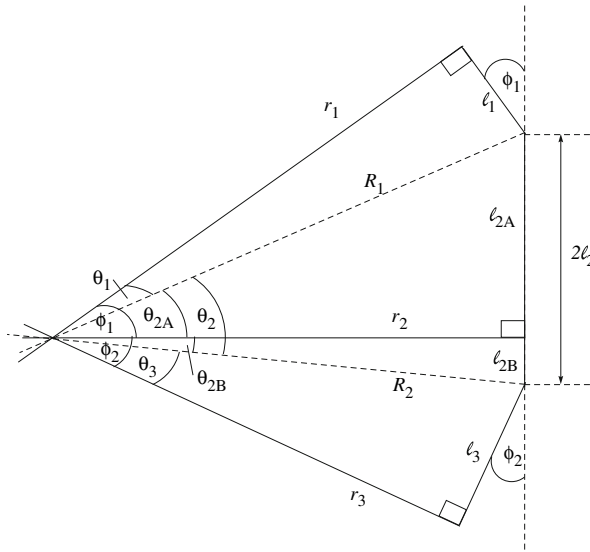**Fig. 3** Elbows formed from three distinct nanotube sections

Given that the parameters $\ell_1, \ell_2, \ell_3, \phi_1$ and ϕ_2 are determined, then the basic repeating unconstrained elbow unit can be obtained and is illustrated in Fig. 3. However, in the case of a nanotorus, we require that an even number of elbow sections forms a symmetrical torus, so that the angles ϕ_1 and ϕ_2 must be constrained to the value $\phi_1 + \phi_2 = 180°/n$ where $n \in \{2, 3, 4, \ldots\}$. So in this case, we minimise the objective function

$$F(\ell_1, \ell_{2A}, \ell_{2B}, \ell_3, \phi_1) = f(\ell_1, \ell_{2A}, \phi_1) + g(\ell_{2B}, \ell_3, 180°/n - \phi_1).$$

In consequence, with this additional constraint, slightly different values for ℓ_1, ℓ_2 and ℓ_3 might be obtained. The resulting nanotorus structure is achieved by translating the elbow in the x-direction by a distance r_2 which is obtained by the procedure which is given in the following section.

3 Model formation for toroidal molecule

Nanotoroidal structures formed from the elbows determined in Sect. 2 are investigated here. We desire to construct and determine a mean radius of the toroidal shapes by connecting the basic elbow units with ϕ_1 and ϕ_2 constrained for the 360° turn. Firstly, we consider the upper quadrilateral, as shown in Fig. 4, which comprises four sides, namely r_1, ℓ_1, ℓ_{2A} and r_2, and the configuration also depend on the angle ϕ_1. On using

Fig. 4 Elbow skeleton formed from three distinct nanotube sections

the compound angle formula for sine, we may deduce

$$\sin \phi_1 = \sin \theta_1 \cos \theta_{2A} + \sin \theta_{2A} \cos \theta_1 = (\ell_1 r_2 + \ell_{2A} r_1)/R_1^2,$$

and therefore,

$$r_1 = (R_1^2 \sin \phi_1 - \ell_1 r_2)/\ell_{2A}. \tag{1}$$

Similarly, from the compound angle formula for cosine, we have

$$\cos \phi_1 = \cos \theta_1 \cos \theta_{2A} - \sin \theta_1 \sin \theta_{2A} = (r_1 r_2 - \ell_1 \ell_{2A})/R_1^2,$$

and therefore we may deduce

$$r_1 = (R_1^2 \cos \phi_1 + \ell_1 \ell_{2A})/r_2. \tag{2}$$

By equating Eqs. 1 and 2, we can rearrange and substitute for r_2 which can be written as

$$r_2 R_1^2 \sin \phi_1 = \ell_{2A} R_1^2 \cos \phi_1 + \ell_1 (r_2^2 + \ell_{2A}^2),$$

where we note that $R_1^2 = r_2^2 + \ell_{2A}^2$ is strictly positive. By dividing by R_1^2 and rearranging, we obtain

$$r_2 = \ell_{2A} \cot \phi_1 + \ell_1 \csc \phi_1, \tag{3}$$

and likewise

$$r_1 = \ell_1 \cot \phi_1 + \ell_{2A} \csc \phi_1.$$

By precisely the same process for the quadrilateral comprising the sides r_2, ℓ_{2B}, ℓ_3 and r_3, we may deduce

$$r_2 = \ell_{2B} \cot \phi_2 + \ell_3 \csc \phi_2,$$
$$r_3 = \ell_3 \cot \phi_2 + \ell_{2B} \csc \phi_2. \tag{4}$$

The parameters ℓ_{2A} and ℓ_{2B} can be rearranged from (3) and (4), respectively, which can be written as

$$\ell_{2A} = \frac{r_2 - \ell_1 \csc \phi_1}{\cot \phi_1} = r_2 \tan \phi_1 - \ell_1 \sec \phi_1,$$

$$\ell_{2B} = \frac{r_2 - \ell_3 \csc \phi_2}{\cot \phi_2} = r_2 \tan \phi_2 - \ell_3 \sec \phi_2.$$

Since $2\ell_2 = \ell_{2A} + \ell_{2B}$, therefore we obtain

$$r_2 = \frac{\ell_1 \sec \phi_1 + 2\ell_2 + \ell_3 \sec \phi_2}{\tan \phi_1 + \tan \phi_2}. \tag{5}$$

By substituting (5) into the above equations, r_1 and r_3 can be obtained

$$r_1 = \ell_1 \cot(\phi_1 + \phi_2) + 2\ell_2 \csc(\phi_1 + \phi_2) \cos \phi_2 + \ell_3 \csc(\phi_1 + \phi_2), \tag{6}$$
$$r_3 = \ell_1 \csc(\phi_1 + \phi_2) + 2\ell_2 \csc(\phi_1 + \phi_2) \cos \phi_1 + \ell_3 \cot(\phi_1 + \phi_2). \tag{7}$$

We comment that these two formulae provide the appropriate generalisation of those given in Cox and Hill [9] for the case of two distinct tubes. The corresponding equations given in Cox and Hill [9] can be formally obtained from (6) and (7) with the formal identification $\ell_2 \equiv \phi_2 \equiv 0$.

Next we attempt to calculate a mean radius a and a mean generating radius c in terms of the perpendicular distances r_1, r_2 and r_3. We utilize the integral formula for a mean radius $\bar{r}$ for a circle which is given by

$$\bar{r}\phi_0 = \int_0^{\phi_0} r(\phi) \, d\phi.$$

For a right-angled triangle which consists of r_1, ℓ_1 and R_1 sides, we have $\phi_0 = \tan^{-1}(\ell_1/r_1)$ and $r(\phi) = r_1 \sec \phi$ and we may deduce

$$\bar{r}_1 \theta_1 = r_1 \int_0^{\tan^{-1}(\ell_1/r_1)} \sec \phi \, d\phi = r_1 \ln \left(\frac{\ell_1}{r_1} + \frac{\sqrt{\ell_1^2 + r_1^2}}{r_1} \right).$$

Since $\sinh^{-1} x = \ln(x + \sqrt{x^2 + 1})$, we therefore obtain

$$\bar{r}_1 \theta_1 = r_1 \sinh^{-1}(\ell_1/r_1).$$

We can repeat the same procedure to obtain the mean radii for r_2 and r_3 and finally by averaging, we obtain the mean toroid generating radius c to be given by

$$c = \{r_1 \sinh^{-1}(\ell_1/r_1) + r_2[\sinh^{-1}(\ell_{2A}/r_2) + \sinh^{-1}(\ell_{2B}/r_2)]$$
$$+ r_3 \sinh^{-1}(\ell_3/r_3)\}/(\phi_1 + \phi_2). \tag{8}$$

We now extend this process to determine a representative expression for the mean tube radius a. Here a surface integral for a torus is undertaken to determine such an average radius. The surface element for the tube is obtained by transforming the toroidal coordinate system (a, ϕ, ψ) into a Cartesian coordinate system given by
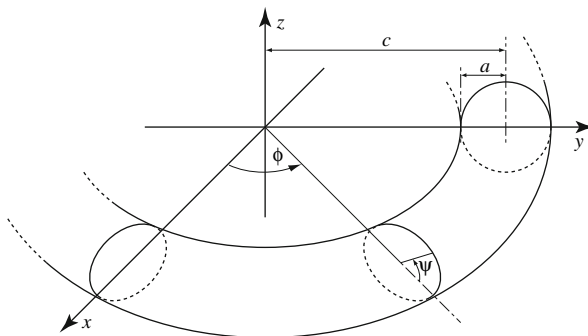
$$x = (c + a \cos \psi) \cos \phi, \quad y = (c + a \cos \psi) \sin \phi, \quad z = a \sin \psi,$$

where c and a denote the mean radii for the torus and the tube, respectively, and ϕ and ψ are the torus and the tube angles, respectively (see Fig. 5). By using the Jacobian matrix, the surface element integral for the torus can then be written as

$$\int_0^{\phi_0} \int_0^{2\pi} b(\phi, \psi)[r(\phi) + b(\phi, \psi) \cos \psi] \, d\psi d\phi = 2\pi \bar{b} \phi_0 c,$$

where $b(\phi, \psi)$ is the radius of the tube and as before $r(\phi)$ is the torus generating radius. For the section of tube A, $\theta_1 = \tan^{-1}(\ell_1/r_1)$, $r(\phi) = r_1 \sec \phi$ and $b(\phi, \psi) = a_1 \sqrt{\sec^2 \phi \cos^2 \psi + \sin^2 \psi}$, we may deduce

$$\bar{a}_1 = \frac{1}{2\pi c \theta_1} \int_0^{\theta_1} \int_0^{2\pi} a_1 r_1 \sec \phi \sqrt{\sec^2 \phi \cos^2 \psi + \sin^2 \psi} \, d\psi d\phi,$$

$$= \frac{a_1 r_1}{2\pi c \theta_1} \int_0^{\theta_1} \int_0^{2\pi} \frac{\sqrt{1 - \sin^2 \phi \sin^2 \psi}}{\cos^2 \phi} \, d\psi d\phi.$$

Fig. 5 Toroidal coordinate system (a, ϕ, ψ)

Upon the substitution of $k = \sin\phi$, the above integral can be written as

$$\bar{a}_1 = \frac{2a_1r_1}{\pi c\theta_1} \int_0^{\pi/2} \int_0^{\ell_1/R_1} \frac{\sqrt{1 - k^2 \sin^2\psi}}{k'^3} dkd\psi = \frac{2a_1r_1}{\pi c\theta_1} \int_0^{\ell_1/R_1} \frac{E(k)}{k'^3} dk,$$

where $E(k)$ is the complete elliptic integral of the second kind with modulus k and $k' = \sqrt{1 - k^2}$ is the complementary modulus. Using these definitions with equivalent expressions for tubes B and C and then combining, we may derive the following formula for the representative tube radius

$$a = \frac{2}{\pi c(\phi_1 + \phi_2)} \{a_1r_1h(\ell_1/R_1) + a_2r_2[h(\ell_{2A}/R_1)$$
$$+ h(\ell_{2B}/R_2)] + a_3r_3h(\ell_3/R_2)\}, \tag{9}$$

where

$$h(x) = \int_0^x \frac{E(k)}{k'^3} dk. \tag{10}$$

The analytical expression in terms of an infinite series for (10) can be found in Appendix A of Cox and Hill [9] which is given by

$$h(x) = \frac{3\pi x}{8r} + \frac{\pi}{8} \sin^{-1} x + \frac{\pi}{2} \sum_{m=1}^{\infty} \binom{-\frac{1}{2}}{m+1}^2 \left\{ \frac{(2m-1)!!}{2^m m!} \sin^{-1} x \right.$$
$$\left. - \frac{x^{2m+1}}{(2m+1)r} \left[1 + \left(\frac{r^2}{x^2}\right) \sum_{k=0}^{m-1} \frac{(m-k-1)!(2m+1)!!}{2^{k+1} m!(2m-2k-1)!!} \left(\frac{1}{x}\right)^{2k} \right] \right\},$$

where $r = (1 - x^2)^{1/2}$ and the double factorial $(2n - 1)!!$ denotes $(2n - 1)$ $(2n - 3) \ldots 5 \cdot 3$. We comment that the above procedures for the determination of the average parameters a and c are by no means unique, but appear as the most natural and simplest for the determination of representative values.

4 Results and discussion

In this section, we begin by considering elbows made from the smallest possible nanotube sections. By precisely the same procedure as that given in [9], the basic parameter for elbows are given in Table 1. The smallest possible nanotube sections which can be formed from the elbows are referred as the base unit, and other possible structures can be obtained by adding further incremental units. We also follow the same nomenclature formulated in [9] for toroidal shaped molecules by utilizing the notation $N(n, m)_p$ where (n, m) refers to a section of nanotube which is constructed from p atoms and N is a number of base units.

Numerical results from the least squares procedure when applied to various distinct nanotube elbows are presented here. We consider two different elbow structures which

are (5,0)–(4,4)–(7,0) and (3,3)–(6,0)–(4,4). Using the new polyhedral facetted model
for carbon nanotubes which incorporates curvature [15] and employing the value of
the bond length $\sigma = 1.42$ Å, the tube radii are obtained. Once the atom positions are
determined, the physical parameters $\ell_1, \ell_2, \ell_3, \phi_1$ and ϕ_2 can be obtained by the
minimisation process, both for no constraints and again with the constraint $\phi_1 + \phi_2 =$
$180°/n$ where $n \in \{2, 3, 4, \ldots\}$. In Table 2, we present the results for the unconstrained
case and the constrainted case when $\phi_1 + \phi_2 = 60°$ where $n=3$ for two different
nanotori. We comment that the sum of the angles ϕ_1 and ϕ_2 needs to be exactly
or close to a common factor of 360° for toroidal structures, and there is only one
case arising for these particular two structures. Moreover, there is no straightforward
procedure to choose the elbow structures for which $\phi_1 + \phi_2 \simeq 180°/n$, so that only
(5,0)–(4,4)–(7,0) and (3,3)–(6,0)–(4,4) are presented here.

Using the parameters for the constrained elbows, we calculate the toroidal parame-
ters r_1, r_2 and r_3 from Eqs. 6, 5 and 7, and finally, values for the mean torus generating
radius c and mean tube radius a are derived from the expressions (8) and (9). These
results are presented in Table 3. Two of these nanotori are illustrated graphically in
Figs. 6 and 7. In Fig. 6, we depict the toroidal structure of $3(5, 0)_{17}6(4, 4)_{48}3(7, 0)_{19}$

**Table 1** Fundamental parameters for nanotube elbows

Nanotube	Radius (Å)	Base unit	Incremental unit	
		Number atoms	Number atoms	Length (Å)
(5,0)	2.0551	17	+20	+4.7986
(4,4)	2.7582	48	+16	+2.4380
(7,0)	2.8094	19	+28	+4.2230
(3,3)	2.0965	12	+12	+2.4206
(6,0)	2.4298	32	+24	+4.1580
(4,4)	2.7582	24	+16	+2.4380

Table 2 Bend angles and base unit section

	Elbow type	
	(5,0)–(4,4)–(7,0)	(3,3)–(6,0)–(4,4)
$\phi_1 + \phi_2$ unconstrained		
$\phi_1 (°)$	25.59	31.38
$\phi_2 (°)$	36.00	33.80
ℓ_1 (Å)	3.7089	3.2202
ℓ_2 (Å)	3.6571	2.4085
ℓ_3 (Å)	3.1727	2.3430
$\phi_1 + \phi_2 = 60°$		
$\phi_1 (°)$	24.00	26.20
$\phi_2 (°)$	36.00	33.80
ℓ_1 (Å)	3.3396	3.2716
ℓ_2 (Å)	3.6571	2.4085
ℓ_3 (Å)	3.1727	2.3430

Table 3 Physical parameters of toroidal structures

Toroidal structures	r_1 (Å)	r_2 (Å)	r_3 (Å)	c (Å)	a (Å)
$3(5, 0)_{17}6(4, 4)_{48}3(7, 0)_{19}$	12.4239	12.7083	13.4038	12.9935	2.6209
$3(3, 3)_{12}6(6, 0)_{32}3(4, 4)_{24}$	9.2163	9.7138	10.1213	9.7980	2.4780
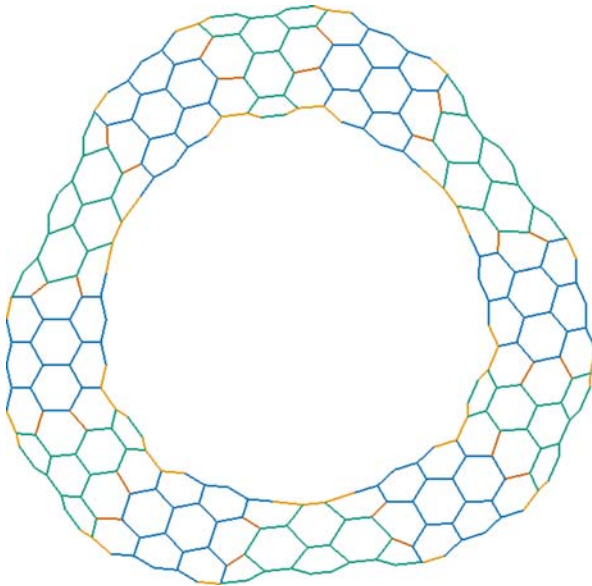
Fig. 6 Nanotorus formed from $3(5, 0)_{17}6(4, 4)_{48}3(7, 0)_{19}$ where $\phi_1 + \phi_2 = 60°$

which can also be referred to as a C_{396} molecule and also in Fig. 7, we show the toroidal structure of $3(3, 3)_{12}6(6, 0)_{32}3(4, 4)_{24}$ which can also be referred to as a C_{300} molecule.

5 Summary

The main contribution of this paper is applying a least squares approach to determine the basic elbow unit and toroidal structures formed from three distinct carbon nanotubes. Within each constituent nanotube structure, the relative atom positions are assumed to remain unchanged. The connection for adjacent atoms on each of the two sections is assumed to be as close as possible to the carbon–carbon bond length, which we take to be $\sigma = 1.42$ Å. We seek to minimise the variation in the bond length which gives rise to the physical parameters, namely the bend angles, ϕ_1 and ϕ_2, and the half-lengths ℓ_1, ℓ_2 and ℓ_3. There are two approaches in the minimisation routines, which are the unconstrained and constrained cases for the bend angles. In terms of the unconstrained procedure, all the physical parameters are allowed to attain their
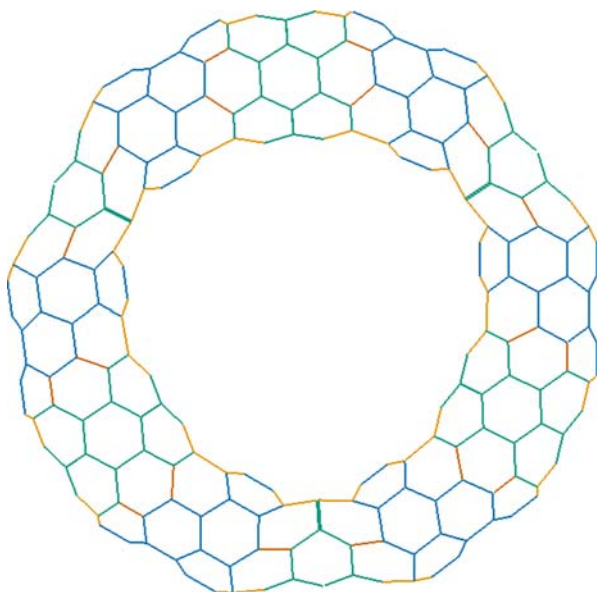
Fig. 7 Nanotorus formed from $3(3,3)_{12}6(6,0)_{32}3(4,4)_{24}$ where $\phi_1 + \phi_2 = 60°$

optimum values themselves which are necessary to form the elbow structures. Howe-ver, in such a procedure, there is no guarantee that the elbow sections can be joined to each other and form a toroidal shaped structure with a 360° turn. Therefore, the ana-lysis is repeated with the angles ϕ_1 and ϕ_2 constrained to the value $\phi_1 + \phi_2 = 180°/n$ where $n \in \{2, 3, 4, \ldots\}$.

Here, we only consider two distinct elbows which are (5,0)–(4,4)–(7,0) and (3,3)–(6,0)–(4,4) and all the physical parameters are given in Table 2. Since the principal aim of the paper is to construct toroidal molecules by joining elbow sections, the bend angles must form a 360° turn. Therefore, we necessarily exploit those elbow sections for which the sum of their bend angles is a factor of 360. We might say that the two elbows which are studied here correspond to cases for which $360/(\phi_1 + \phi_2)$ approximately is an integer.

Following the analysis of two elbow types, we then consider toroidal shaped molecules. We establish a straightforward procedure to determine the mean gene-rating toroidal radius c and the mean tube radius a. Once the bend angles and tube lengths are obtained, the perpendicular lengths from the torus centre can be deter-mined as given in Table 3. We comment that such theoretical structures have yet to be confirmed either experimentally or by molecular dynamics simulations. However, their theoretical existence is a first step in understanding the complex geometrical structures of such molecules.

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