

Elemental Benzenoids

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Received May 18, 1993*

Attention is directed to the conceivable possibility of finite-sized "elemental benzenoids" comprised solely from carbon atoms, every one of which is located only in hexagonal rings. To avoid hydrogens at boundaries, the polyhex structure then must be embedded in a finite closed surface. Mathematically there are exactly two possibilities for such surfaces: the torus and the nonorientable surface of cross-cap number 2, with the torus presumably of more chemical relevance since only it embeds into Euclidean 3-space without self-intersection. For either type of surface a systematic possibly comprehensive identification scheme is developed for consequent stereoisomeric structures, oftentimes many of which correspond to a single constitutional isomer.

1. INTRODUCTION

There has long been interest in novel carbons. Indeed there are many elemental carbons which, though presumably somewhat "graphitic", are really poorly characterized at the atomic scale—such examples being found in most issues of the journal *Carbon*. At larger scales there are many unusual morphologies: fibrous¹ and even toroidal.² At the atomic scale the recent discoveries of stable elemental carbon cages³ as well as of nanotubes⁴ have engendered much interest in other possibilities for carbons. Indeed theoretical suggestions,^{5,6} of novel elemental carbon structures predate this recent interest, even with regard to the consideration⁶ of the truncated-icosahedron structure of "Buckminsterfullerene". In the more traditional organic chemical field there has been a long-standing interest in *benzenoid* systems comprised of planar polyhex carbon networks, which however are not elemental in having hydrogen atoms at their boundaries. Graphite of course may be viewed as the limit where the boundary fraction (of atoms) falls below some tolerance limit, and what the boundary is like is usually neglected.

Here an investigation is begun to determine the possibilities for finite *elemental benzenoids*, these being viewed as finite π -conjugated networks formed solely of carbon hexagons fused in such a way so as to have no boundary. It is sought at least to outline a comprehensive approach to *all* conceivable possibilities, as dictated via a few fundamental mathematical results from the fields of topology and graph theory. In fact already for one of the two general classes, namely, that of toroidal benzenoids, there is some work⁷⁻¹⁰ on a limited subset of these species. The aim here is to identify the full range of possibilities indicating how the conceivable structures fit into conventional stereochemical theory, e.g., as discussed in ref 11. Too the consideration of toroidal benzenoids relates to the theory of nanotubular carbon polymers (i.e., buckytubes), as have been much investigated since their experimental realization—indeed the (simpler) characterization of the structural possibilities for these *infinite* toroidal benzenoids has already been completed.¹²

2. STOICHIOMETRY AND TOPOLOGY

Given a number v of carbon atoms forming an elemental benzenoid, they are to be embedded in a surface \mathcal{S} , and each carbon is linked by σ -bonds so that all rings (or faces) on \mathcal{S}



Figure 1. Sphere with one handle (so that its genus is 1) and thence homeomorphic to a torus.

are hexagonal. To avoid boundaries (and consequent hydrogen atoms), the surface \mathcal{S} is closed. Since each carbon is in three rings while each ring contains six carbons, the number of (hexagonal) faces must be

$$f = v/2 \quad (2.1)$$

and a similar argument reveals that the number of edges (or σ -bonds) must be

$$e = 3v/2 \quad (2.2)$$

Evidently v must be even.

A further significant topological result is that for a network embedded in a surface \mathcal{S} an Euler relation applies

$$v - e + f = \chi(\mathcal{S}) \quad (2.3)$$

where the *Euler characteristic* $\chi(\mathcal{S})$ is an integer topological index which is invariant under any smooth topological transformation (i.e., homeomorphism) of \mathcal{S} . (See any of a number of texts, such as ref 13, 14, or 15.) For an "orientable" surface \mathcal{S} this invariant takes the form

$$\chi(\mathcal{S}) = 2 - 2g(\mathcal{S}) \quad (2.4)$$

where $g(\mathcal{S})$ is the surface's *genus*, this being the number of handles attached to a sphere's surface to make it homeomorphic to \mathcal{S} . (See Figure 1.) On the other hand, for a "nonorientable" \mathcal{S} ,

$$\chi(\mathcal{S}) = 2 - n(\mathcal{S}) \quad (2.5)$$

where $n(\mathcal{S})$ is the surface's *cross-cap number*, this being the number of cross-caps placed onto a sphere's surface to make it homeomorphic to \mathcal{S} . See Figure 2. As first argued by Dyck¹⁶ in 1888, all possible closed surfaces \mathcal{S} are so obtained with addition either only of handles or only of cross-caps to a sphere. If both occur on a sphere, then a cross-cap and handle together turn out to be topologically deformable (i.e., equivalent) to a triple of cross-caps. The rigorous establishment of this classification is due to Dehn and Heegard¹⁷ and also is described in section 1.3 of the text of ref 15.

* Abstract published in *Advance ACS Abstracts*, March 15, 1994.

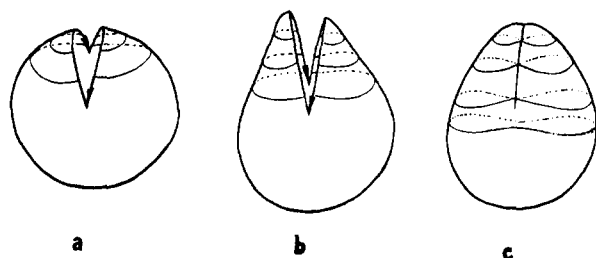


Figure 2. (a) Hollow sphere with a slice in its surface, the two edges of the cut each having an arrow along the edge as indicated. Gluing the two edges back together such that corresponding parts of the two arrows join (head-to-head and tail-to-tail), as indicated in b and c results in a cross-cap and a surface (the "projective plane") with $n(\mathcal{S}) = 1$.

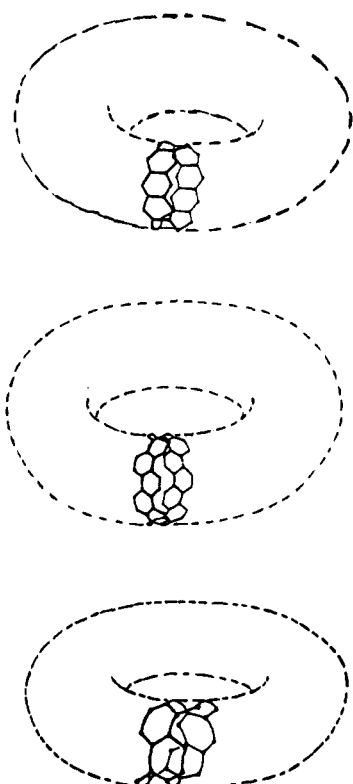


Figure 3. Three possible types of embeddings such that when the indicated unit cell is iterated around the torus a polyhex covering is obtained.

For the present case eq 2.1 and 2.2 when substituted in (2.3) imply that

$$\chi(\mathcal{S}) = 0 \quad (2.6)$$

As a consequence there are exactly two topological classes of surfaces which might give rise to elemental benzenoids: the orientable case

$$g(\mathcal{S}) = 1 \quad (2.7)$$

corresponds to a *torus*, while the nonorientable case

$$n(\mathcal{S}) = 2 \quad (2.8)$$

corresponds to a *Klein bottle* (named after the famous German mathematician and geometer Felix Klein¹⁸). A few possibilities for embedding on a toroid \mathcal{S} are indicated in Figure 3. For the Klein bottle one has a situation indicated in Figure 4, where in fact the surface (when embedded in 3-space) must intersect itself. Rather amusingly, chemistry offers some conceivable possibility for tolerating such self-intersections,

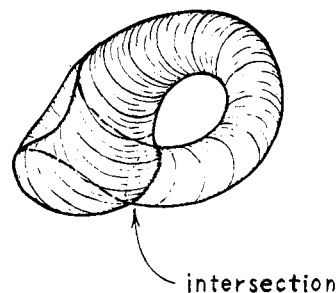


Figure 4. One of the "simplest" closed surfaces with but one side, this having $n(\mathcal{S}) = 2$. The two portions of the surface intersect along the dotted line indicated.

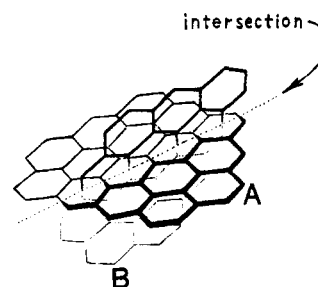


Figure 5. Possible scheme for the "self-avoiding" intersection of two portions A and B of hexagonal net.

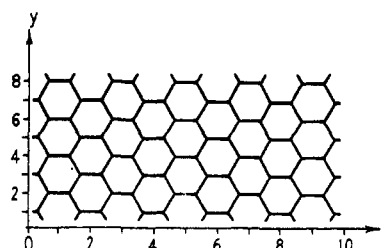
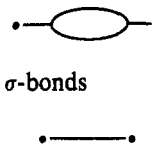


Figure 6. $L \times w$ section of the honeycomb lattice with $L = 10$ and $w = 8$.

as indicated in Figure 5. There, the bonds on one portion A of \mathcal{S} are to pierce the centers of rings of the B portion of \mathcal{S} , and conversely. Space-filling models suggest that this "trick" should probably be of excessively high energy. But, if the edges of the network are taken as acetylenic (or allenic) linkages with a set of σ -bonds



in place of individual σ -bonds



then the rings are much bigger and self-intersection should be sterically allowable. Of course with such a replacement the species would not be a usual benzenoid, though networks based upon such a replacement have been studied.¹⁹ Also other possibilities²⁰ for Klein bottles have been considered (also possibly using polyyne chains).

3. STRUCTURE CONSTRUCTION FOR TORI

One way to obtain toroidal benzenoids is to view them by cutting suitable rectangular sections from the graphite (or honeycomb) lattice. Such an $L \times w$ section is shown in Figure 6. Then one can imagine corresponding bonds within the strip approaching $y = 0$ from above and $y = w$ from below, being joined (i.e., coinciding) while a similar joining of bonds

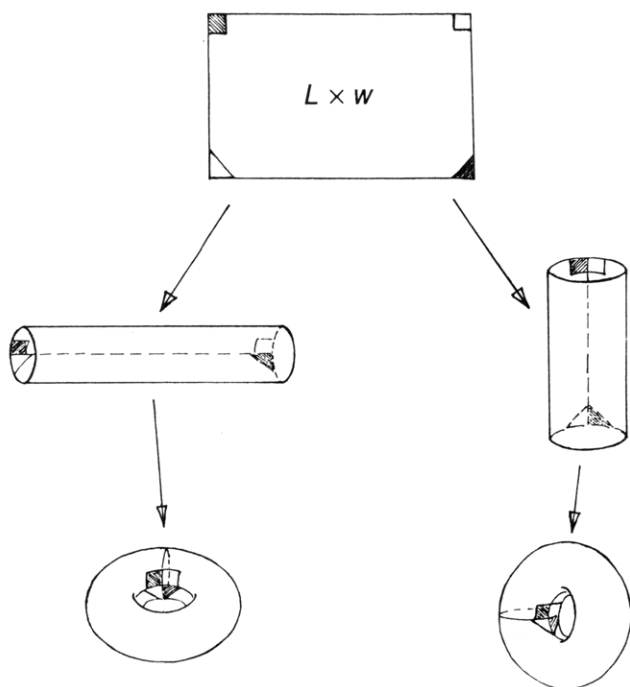


Figure 7. Two ways of forming a rectangular section of network (as from Figure 6) into a torus, while maintaining the same connection pattern of bonds.

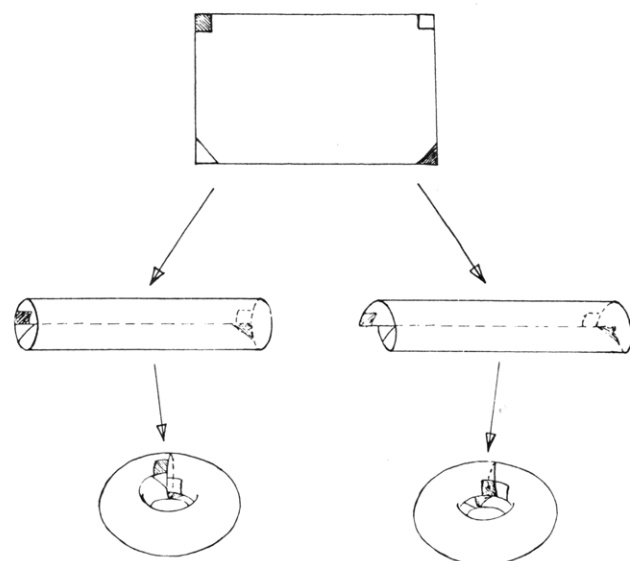


Figure 8. Two possible types of twistings formed as in the left-hand manner of Figure 7.

at $x = 0$ and $x = L$ is made. For a given rectangular section two possible tori can be constructed as indicated in Figure 7. But since the same bonds are sewn together in each circumstance, the *graph* is the same. That is in a classical chemical sense the two toroidal species have the same connectivity pattern (sometimes referred to as the same chemical structure). Thus the two species are distinct *stereoisomers*, though they are not distinguished as “constitutional” (or structural) isomers.

Beyond the two (graph-isomorphic) patterns of sewing together edges of the rectangle of Figure 6, there are two other twisted possibilities indicated in Figure 8. That is, the i th bond along one edge is made to coincide with a “shifted” bond at position $i + m$ along the opposite side. In general the parity of m must correlate in a certain manner with the parity of the corresponding length L or width w . That is, for odd

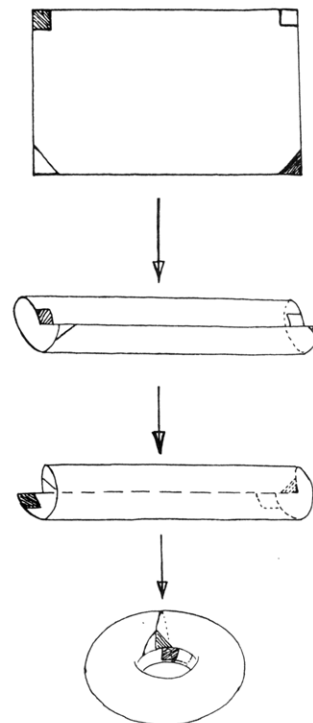


Figure 9. Another way of forming a torus, with inside and outside interchanged.

length (and even width) the horizontal bonds at the left and right extremes are located at even and odd vertical positions, so that there must be a shear m between the bonds at $x = 0$ and $x = L$ such that m is odd. For odd width (and even length) there must similarly be a shear between bonds at $y = 0$ and $y = w$ which is odd. For the case of Figure 6 where both L and w are even, the shear must be even, though it can be either along the horizontal or vertical sewing together of edges.

Beside the 2-fold choice of Figure 7 and the multifold choice for shear as in Figure 8, there is another 2-fold choice regarding the inside and outside of the torus. For example instead of making the construction on the right-hand side of Figure 8, the construction with the interchange of inside and outside could be made as in Figure 9. The result though joining the same bonds (and thereby yielding the same graph and constitutional isomer) is embedded in space in a different topological manner. But examination of the result reveals that what has been obtained is a torus of corresponding negative shear. That is, the inside–outside reversal does not produce new tori if we allow both negative and positive (or left and right) shear.

Further, the question now arises whether it is possible to make “nontrivial” *simultaneous* shears along the horizontal and vertical directions. The answer is yes! But to do so we need to utilize a suitable nonrectangular fragment from the honeycomb lattice, such as that indicated in Figure 10a. Here dangling bonds at the left and right ends are to be joined, as well as dangling bonds at the top and bottom, all according to the manner indicated in Figure 10b. That is, dangling bonds at correspondingly labeled portions of the boundary are to be joined such that the indicated arrows match (head-to-head and tail-to-tail). For this doubly twisted ($mn \neq 0$) case, there, however, are two parity constraints, the first dictated by the condition that the “type” of corner at the upper left match to the type of corner in the notch (at the lower right) and next that dictated by the similar matchings after forming the tube with attachments made along the m

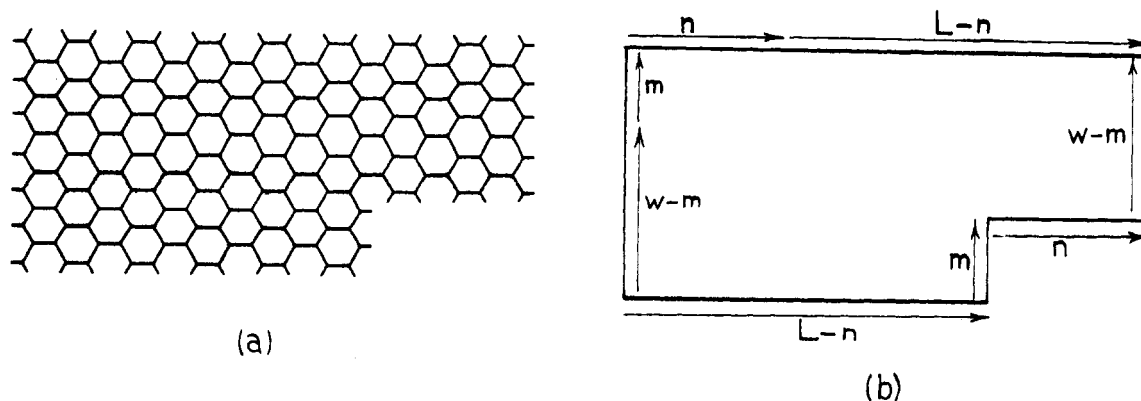


Figure 10. Fragment of the graphite lattice in a to be used in constructing a "doubly-twisted" polyhex torus, where the pastings (or bond joinings) to achieve the torus are indicated by corresponding labels in b.

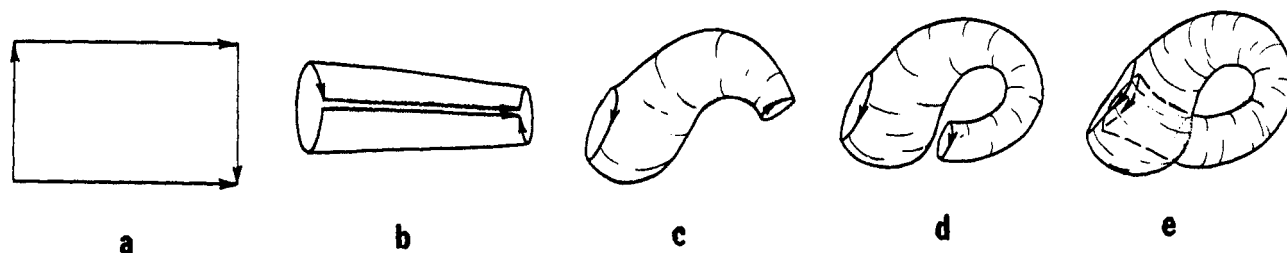


Figure 11. Step-by-step formation of a Klein bottle starting from a rectangular sheet, as in a with opposite directed edges of the rectangle to be adjoined such that arrows match head-to-head and tail-to-tail. The puncturing of the surface occurs between d and e, and the final bottle, which would be f, is shown in Figure 4.

and n edges of Figure 10. After a little experimentation one finds that w and m are to be of opposite parities, as also must be the case for L and n . Further if the twist m is negative (and $n > 0$), the "empty notch" of Figure 10 would appear instead in the upper right-hand corner; and if the second twist $n < 0$, then the "empty notch" would be shifted from the right-hand to the left-hand side. The torus so constructed in accordance with Figure 10, we denote by $T_{m,n}(L,w)$, where $|m| < w$, $|n| < L$, and the parities of m and w correspond as do those of n and L . As perhaps is most easily seen for a single twist (i.e. for $mn = 0$), though the twists may be increased in magnitude beyond the given limits, it is just that the shape of the honeycomb fragment depends only on m of a fixed sign in a w -modular fashion and on n of a fixed sign modulo L . Such additional full-cycle twists, a in number for the m -direction and b in number for the n -direction, will be indicated by superscripts, thusly, $T_{m,n}^{a,b}(L,w)$. If the superscript is omitted it is understood that $a = b = 0$. Of course, for each graph two embeddings on the surface of a torus are possible, as indicated in the first paragraph (and Figure 7) of this section.

4. STRUCTURE CONSTRUCTION FOR KLEIN BOTTLES

For a Klein bottle elemental benzenoids can be obtained by similar constructions starting from different sized sections, much like that for the torus. Most simply the section is rectangular ($L \times w$ as in Figure 6) with the top and bottom edges to be adjoined as for the torus. The difference then comes at the left and right edges where bonds at corresponding positions along the arrows at the left- and right-hand sides of the rectangle in Figure 11a are to be adjoined. The consequent construction illustrating the necessity of puncturing the surface to match these two arrows is shown in later parts of this figure. In a more algebraic vein, the first class of structures $K_{m,0}$

(L,w) results from identifying corresponding (equal- x) bonds at $y = 0$ and $y = w$, while also identifying bonds i at $x = 0$ with bonds $w + m - i$, modulo w , at $x = L$. Again the parity of m and L are to match. Instead of joining first the top and bottom followed by the "convoluted" joining of left and right edges, these joinings might be done in the opposite order. First for $m = 0$ carry out the convoluted joining at the left and right, whence a smooth-edged Möbius strip is obtained, and an arbitrary twist may be made for the "horizontal" edge to give $K_{0,n}(L,w)$. The construction is indicated in Figure 12a. Moreover this can be elaborated to lead to a construction for "doubly-sheared" Klein bottles: a shifted ($m \neq 0$) convoluted twist is (partially) made as in Figure 12b; then before joining the "horizontal" edge instead a little $n \times m$ section of strip is added as in Figure 12c; and finally the horizontal edge is joined up with the two kinks matching together, thereby giving $K_{m,n}(L,w)$. As for the doubly-twisted tori, attention needs to be paid to parity-mediated matching constraints. The convoluted twist at the vertically oriented edges could also be made at the horizontally oriented edge, whence structures we denote with a superscript asterisk result: $K_{m,n}^*(L,w)$. Twists by more than one full rotation could also be imagined whence also superscripts a, b would be added.

5. ISOMERISM AND ISOTOPY

Questions now arise as to whether all possible stereoisomers have been obtained, as to whether any stereoisomers have been duplicated, and as to which stereoisomers have the same connection pattern. Here by "connection pattern" we understand the molecular *graph* (of the σ -bonded network), which then identifies a structural (or constitutional) isomer. By stereoisomer we here understand what is termed¹⁵ a topological *isotopy* equivalence class of embeddings of a network such as in Figure 6 into a surface \mathcal{S} (here either a torus or a Klein

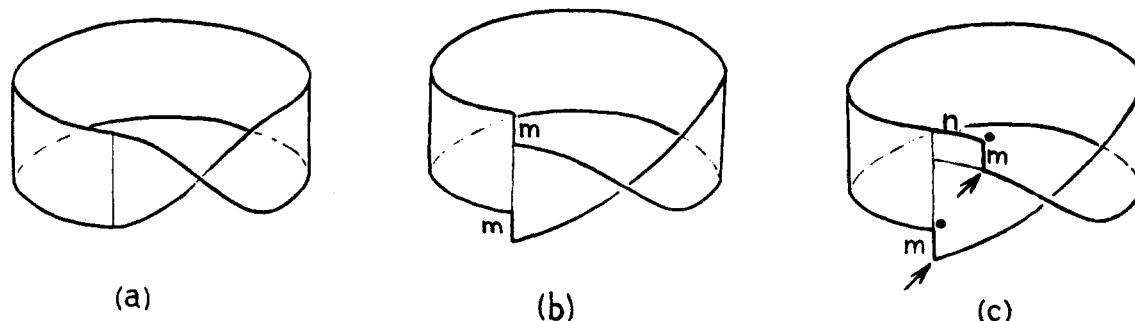


Figure 12. Möbius strips arising as intermediates in the construction of doubly-twisted Klein bottle embeddings. In forming the Klein bottle the two corners (convex and concave) marked by arrows in c are to be matched together, as are the two corners marked by dots.

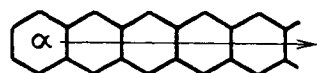


Figure 13. Ring α (on \mathcal{S}) and the beginning of an acenic (parafused) strip of hexagons.

bottle). More precisely two embeddings of a network (comprised of vertices and interconnecting bonds) are isotopy equivalent, if one embedding can be continuously deformed within \mathcal{S} into the other without the coincidence of any parts (vertices or bonds) of the network with one another.

A few side comments on topological equivalencies might be made. If the constraint of the avoidance of coincidences within \mathcal{S} is dropped from the definition of isotopy, then the resultant common topological equivalence is called *homotopy*. That is, in homotopy equivalence a geometric object (here our network) can be continuously deformed, "lifting" it out of any surface \mathcal{S} it might initially be in — or even lifting it out of Euclidean 3-space \mathcal{E}_3 . Evidently homotopy equivalence of our networks nearly corresponds to graph isomorphism. Though for embeddings in two-manifolds (as here) the two equivalences evidently can sometimes²¹ coincide, it is imperative for the present purposes to keep different parts of the network from collapsing into one another. To distinguish embeddings in \mathcal{S} with \mathcal{S} itself embedded in (the ambient) Euclidean 3-space in either of two possible ways, as in Figure 7, is, however, a more delicate matter. One demands that the deformation (i.e., homeomorphism) be extendable to all of the (ambient) space \mathcal{E}_3 . The resultant¹⁵ ambient isotopy equivalence classes distinguish the two cases of Figure 7, and also for the Klein bottle it distinguishes different ways of "interlacing" links through ring centers (as indicated in Figure 5).

The notion of topological equivalences bears further on how the surface \mathcal{S} is in turn embedded in \mathcal{E}_3 . The torus \mathcal{S} is a cylinder joined at the ends, much like the outer boundary of a piece of finite-diameter cord joined at the ends into a loop. But the cord, and thence also \mathcal{S} , can be knotted. Here the relevant topological concept is isotopy classes of embeddings of \mathcal{S} in the ambient \mathcal{E}_3 space and is a topic well-developed in the mathematical literature as the area of *knot theory*. See, e.g., ref 22. The additional overall classes (and stereoisomers) so arising are identified by a pair of independent labels: one for the embedding of the polyhex in \mathcal{S} and one for the knotting of \mathcal{S} in \mathcal{E}_3 . Here (it is seen), we focus on the first of these independent embedding problems.

That all possible graphs (i.e., structural isomers) have been identified at least for the toroidal case can be proved. Given an arbitrary covering of \mathcal{S} by hexagons, one chooses a particular hexagon α , as in Figure 13, and then proceeds from it to a neighboring hexagon and thence along an acenic (parafused) path, until one arrives at a hexagon ω already visited. This

construction,²³ which we call an "Altshuler construction" as applied for the torus, reveals after careful argument the consequent polyacenic cycle even has ring ω parafused, the ring α is the same as ω , and the polyacenic cycle is not Möbius twisted. Even numbers of half-twists in the polyacene cycle may occur but are graphically (or homeomorphically) equivalent to the untwisted case. Now extension of such an h -hexagon cycle to include the neighbor rings to the polyacenic strip with a number h of hexagons, then next their neighbors, and so forth ultimately leads to a graph identical to one of the class $T_{m,0}(L,2h)$. Here it is understood that the special case where the polyacenic cycle is a neighbor to itself is allowed, in which case $L = 1$. The more complicated case of polyhex coverings on a Klein bottle is given some consideration in ref 24.

6. GRAPH ISOMORPHISM OF STEREOISOMERS

There remains the question as to which toroidal structures have the same graph. Clearly there must be many such occurrences since we have just noted all the graphs are found among the subset of toroidal benzenoids of the type $T_{m,0}(L,2h)$. Here we indicate some partial results, without going into very much detail in the derivation of these results. First, if we imagine a construction such as on the right-hand side of Figure 8, a twist at the final stage through 2π radians (or any integral multiple thereof) before the final joining clearly leads to the same graph, and a similar comment applies to shears along the other direction. Thus

$$T_{m,n}^{a,b}(L,w) \approx T_{m,n}^{0,0}(L,w) = T_{m,n}(L,w) \quad (6.1)$$

For chemically feasible (i.e., not inordinately strained) structures it is anticipated that $L \gg w$ (for foldings as in Figure 8, or on the left in Figure 7), whence longitudinal twists should not occur, i.e., $b = 0$. Further such considerations suggest that $|a|$ should not be too large compared to L/w . Now reflection or inversion of a structure leads to

$$T_{m,n}^{a,b}(L,w) \approx T_{-m,-n}^{-a,-b}(L,w) \quad (6.2)$$

There are additional equivalences based upon the choice of different directions for the polyacenic path of Figure 13. For the cases where the torus is based upon a rectangular section (i.e., with $mn = 0$) the results of such different choices are more readily determined. For $n = 0$ such an Altshuler construction in an alternative direction leads (as indicated in the appendix) to

$$T_{m,0}(L,w) \approx T_{m,0}(w/2p,2pL) \quad (6.3)$$

where

$$p = w/\gcd\{L + m, w\}$$

$$m' = 2rL + w/2p \quad (6.4)$$

with r defined as the solution to

$$r(L + m) = -w/p, \text{ mod } w \quad (6.5)$$

For the case $m = 0$, a similar sort of equivalence may be established

$$T_{0,n}(L, w) \approx T_{m',0}(L/2p, 2wp) \quad (6.6)$$

where

$$p = L/\gcd\{w + m, L\}$$

$$m' = 2rw - 3L/2p \quad (6.7)$$

with r defined as the solution to

$$r(w + m) = L/p, \text{ mod } L \quad (6.8)$$

The four transformations indicated in (6.1)–(6.3) and (6.6) thence generate a group and form a set of stereoisomer structures all corresponding to the same graph (or structural isomer). Correspondences such as (6.3) and (6.6) for the doubly-twisted case ($mn \neq 0$) have not yet been made.

The analysis for the Klein bottle has many parallels, but so far the analysis¹⁸ is less complete. By much the same reasoning as that which led to (6.1) and (6.2), one finds

$$K_{m,n}(L, w) \approx K_{m,n}^{a,b}(L, w) \approx K_{-m,-n}^{a,b}(L, w) \quad (6.9)$$

There are of course some sort of correspondences analogous to (6.3) and (6.6) too, as well as correspondences for the alternative class $K_{m,n}^{a,b*}(L, w)$. But even after this there arises an ambient isotopy problem upon embedding in Euclidean 3-space whence one pays attention to the topological detail of the self-intersection of the surface.

7. CONCLUSION

As seen here, there is a wide range of mathematical possibilities for elemental benzenoids which are shown here to occur exclusively as embeddings of polyhex carbon networks in either the torus or Klein bottle. The circumstances for such carbon-network embeddings bear some points of contradistinction to the case of embeddings in spherical (or many other) surfaces. First for the sphere, rings of other (smaller) sizes are required e.g., as noted in ref 7. Second for the sphere there is²⁵ but one embedding (not distinguishing mirror images) of a carbon network, while for the torus and Klein bottle there

are many topologically distinct embeddings, and therefore many conceivable chemical isomers with the same connection pattern (or graph). Such stereoisomers thence are “topological” in somewhat the same sense as knotted molecules—neither would be isomers were chemistry in four dimensions. In any event the comprehensive topological specification of elemental-benzenoid structures is here much more nearly complete (analytically) than that for fullerenes, on the surface of a sphere (this latter case so far being done²⁶ only for restricted vertex counts in a brute-force computer-intensive manner). Here we conjecture that (especially for the more chemically relevant torus) all topological isotopy equivalence classes of structures (corresponding to stereoisomers) have been found. Of course as noted following eq 6.1, some classes correspond to overly strained structures. This occurs particularly for Klein bottles at the region of intersection (though there remains some possibility of related nonbenzenoid structures, noted in connection with Figure 5). Excessive straining occurs also when w is too small, even with small twist m . (Indeed for “nonphysical” very small w or L , some anomalies violating our assumptions can occur, e.g., for $w = 1$, $m = n = 0$ the hexagon(s) on each side of a bond can be the same one.) Further in the proposed classification, some equivalence classes might be duplicated, by different $T_{m,n}^{a,b}(L, w)$ or $K_{m,n}^{a,b}(L, w)$ or $K_{m,n}^{a,b*}(L, w)$ labels. The Altshuler construction shows that at least for the torus all graphs (i.e., constitutional isomers) have been obtained. Moreover at least at the graph-theoretical level this construction reveals a very high symmetry for toroidal benzenoids, namely, unit cells can be taken to contain just a pair of sites, much like that for¹² the infinite “buckytubes”.

The development here of a systematic possibly comprehensive identification for consequent stereoisomeric structures corresponding to topological equivalence classes indicates a wide range of novel possibilities. These consequent possibilities enrich the conventional¹¹ range of stereochemical structures.

ACKNOWLEDGMENT

Several people have made helpful comments, including Drs. A. T. Balaban, R. Bendale, M. Cravey, S. J. Cyvin, X. Liu, P. G. Mezey, V. Nicholson, M. Randić, Ch. Rücker, H. Sachs, T. G. Schmalz, W. A. Seitz, D. Sumners, J. Szucs, N. Trinajstić, H. Zhu, and R. Zoellner. Support of the research is acknowledged to the donors of the Petroleum Research Fund, administered by the American Chemical Society, and to The Welch Foundation of Houston, Texas.

APPENDIX

The object here is to derive 6.3–6.5, identifying different toroidal benzenoids which nevertheless have the same graph.

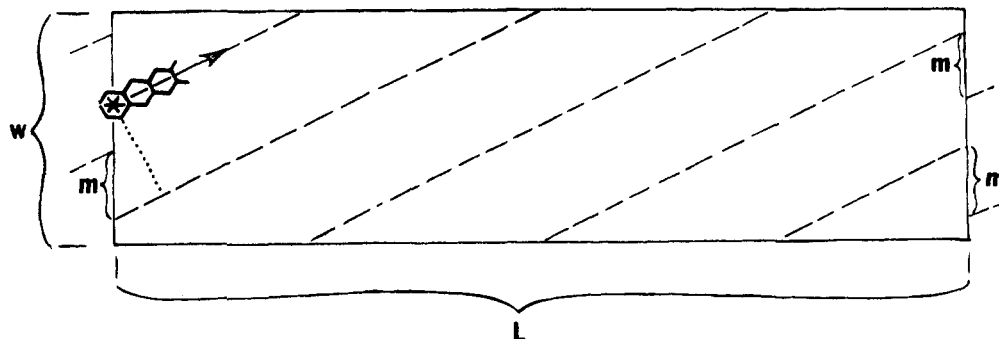


Figure 14. Example rectangle to be formed into a toroid. A polyacenic Altshuler path is indicated by the dashed line, which in our displayed example winds $p = 2$ times around in the horizontal direction and $q = 3$ times around in the vertical direction. The new L' direction from the asterisk (discussed near and following eq A.4) is indicated by a dotted line.

The polyacenic Altshuler path winds around the torus $T_{m,0}(L,w)$ some numbers, p and q , of times in the horizontal and vertical directions (when one views the toroidal surface sliced open as a rectangle). See, e.g., Figure 14. If the number of steps (i.e., the number of hexagons) in such a path is denoted by N , then

$$\begin{aligned} N &= pL \\ N + mp &= qw \end{aligned} \quad (\text{A.1})$$

Consequently, upon elimination of N ,

$$p(L + m) = qw \quad (\text{A.2})$$

In fact this is directly seen if we note that the vertical shift by m readjusts the polyacenic path in much the same manner as would occur with a horizontal length of $L + m$ (and no shift). Since interest is in the first return of the polyacenic path to its starting point, we seek the smallest (nonzero) integer solutions of (A.2) for p and q . Thus letting d denote the greatest common divisor (or gcd) of $L + m$ and w , we have

$$\begin{aligned} p &= w/d \\ q &= (L + m)/d \end{aligned} \quad (\text{A.3})$$

But another embedding of the same graph with the same polyacenic cycle may be made with this polyacenic walk in the vertical direction. This walk with pL hexagons would correspond to a width of $w' = 2pL$, and in order to make the total number of hexagons in the whole torus $Lw/2$, the new length would need to be $L' = w/2p$. That is, we have

$$T_{m,0}(L,w) \approx T_{m',0}(w/2p, 2pL) \quad (\text{A.4})$$

with m' some appropriate twist on the new toroid. This new twist m' may be derived from the original toroid (as in Figure 14), noting that the new L' direction is perpendicular to the selected polyacenic Altshuler path. If leaving in the L' direction from the initiating hexagon marked with an asterisk (and counted as ring 0), one first encounters the Altshuler path again at ring-count position M ; then evidently $m' = 2M$. To determine M , we note that in proceeding from the asterisk to M along the Altshuler path, one winds around the vertical and horizontal directions some numbers of times, r and s . Then the changes in position between the asterisk and M in the vertical and horizontal directions (as measured on the original toroid rectangle) should be

$$\begin{aligned} M - rL &= L'/2 \\ M + rm - sw &= -3L'/2 \end{aligned} \quad (\text{A.5})$$

Consequently upon elimination of M

$$r(L + m) - sw = -2L \quad (\text{A.6})$$

or recalling that $L' = w/2p$

$$r(L + m) = -w/p, \text{ mod } w \quad (\text{A.7})$$

Thus

$$m' = 2M = 2rL + L' - 2rL + w/2p \quad (\text{A.8})$$

and we have accomplished our goal.

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