Aspects of topology, genus and isomerism in closed 3-valent networks

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Recent work on toroidal and Klein bottle fullerenes is reported, including, in particular, attempts to generate useful visual models with the NiceGraph program (part of the Vega package). Some strengths and weaknesses of this modelling software are mentioned. The so-far-unanswered question of what ratio of small radius (r) to large radius (R) might be preferred by a geometric realisation of a toroidal network, and broad categories of isomerism are briefly discussed.

1. Introduction

Toroidal fullerene graphs are regular (cubic) graphs that can be embedded in the surface of a torus (figure 1). The corresponding molecules have been recognised as occurring in a real physico-chemical process only very recently [41]. However, the properties of such hypothetical structures have been studied or reviewed in a number of papers [1–3,6,7,14–27,29–31,33–40,48,50–57].

They are worthwhile objects of study for several reasons. For example, their geometry is quite different from that of the now-conventional topologically planar fullerenes and might afford new opportunities for catalysis (by new opportunities for holding reactive substrates in position). Unlike buckminsterfullerene and its relatives, that need the presence of twelve pentagonal faces, toroidal species can be completely tessellated by hexagons. Although feasible structures would need to be quite large (300 or more carbon atoms at least), they would be smaller than most graphite monolayers, but, being boundless, are likely, in some respects at least, to resemble infinite graphite sheets. Molecular scale semi- and super-conductors with interesting properties might emerge. Here we briefly summarise our current knowledge of such structures, and report recent efforts to obtain satisfactory visual models.

Klein bottle fullerenes [31,37–40,56] too, can be constructed of hexagons alone, and they have been briefly examined before. They require their surfaces to self-intersect, and so have additional complications. Here too we report some successes and failures in our attempts to create plausible structure drawings with 3D perspective.
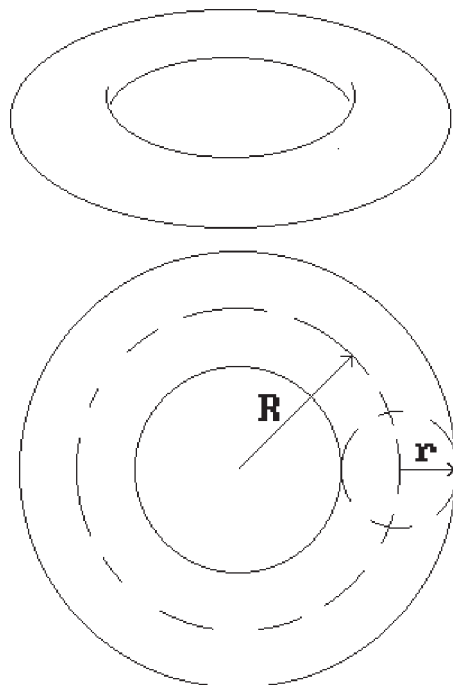
Figure 1. A torus, in perspective and in plan view, showing the characteristic radii r and R used to define it.

Mathematical objects such as the torus and Klein bottle can, of course, be satisfactorily represented as pure topological objects without any reference to the geometric embedding of the objects in space. For example, they can be regarded as infinite doubly periodic planar mappings in order to deduce their formal mathematical properties. However, this is of limited help in gaining the 'visual and tactile' kind of appreciation of structure that is so necessary for real chemistry, and there is no substitute for models that show spatial as well as connectional relationships in three dimensions, and, preferably, that can be rotated for viewing from different angles.

Several very promising methods for visualisation [8] (Kamada–Kawai (KK) [28], Fruchterman–Reingold (FR) [12], and adjacency matrix eigenvectors (AME) [10,13,44]) have recently been developed. These complement traditional molecular mechanics methods by providing a set of vertex coordinates that are plausible enough to provide a helpful drawing, and can in addition be used as a good starting approximation for more sophisticated calculations. An implementation of these NiceGraph methods forms part of the Vega package [46]. Here we have used mainly the Fruchterman–Reingold algorithm, implemented for DOS in a program called VIEW.EXE developed by B. Plestenjak. In this model, functions of distance-to-some-power are selected. Then a repulsive force (α 1/distance^p) between every pair of vertices and an attractive force (α distance^q) between every adjacent pair are calculated. The algorithm calculates the static equilibrium state in which resultant forces for all vertices are reduced to zero.

2. Toroidal fullerenes

For practical purpose, these fall into two classes; namely, toroidal polyhexes, in which the only kind of face is a hexagon, and toroidal fullerenes or 'torusenes' of mixed ring sizes. In the former case, isomers differing in connectivity may conveniently be characterized and enumerated by arrays of three integers [34].

A computer program has recently been developed for this [36], and in many cases it can also generate connection tables and eigenvalues. Toroidal fullerenes of arbitrary ring size are much more intractable, and no general method for their construction, corresponding to the polyhex method, or like the Bielefeld workers' very powerful algorithm for fullerenes [4], yet exists. In general for these cases, *ad hoc* construction methods must be used, and modification of a preformed polyhex of known structure is a convenient approach.

Toroidal polyhexes have some interesting mathematical properties which suggest that they are indeed likely to resemble graphite more than either conventional fullerenes or finite planar benzenoids. For example:

1. The leapfrog transformation[1] [9,45] performed on fullerenes generates closed shell structures, whereas leapfrogs of toroidal polyhexes form only open shell structures [58].

2. Certain toroidal polyhexes can be fully benzenoid (their structure can be formulated as a set of disjoint hexagons that account for all the vertices; see figure 2(a)). However, unlike the case with finite planar benzenoids, *which* set of hexagons is used for the covering (the 'full' set) is not unique – in these toroidal structures one can start the covering of vertices from any hexagon. Furthermore, and again unlike finite planar benzenoids, it is possible for such a polyhex to be fully-arenoid in more than one sense, for example, to be both fully benzenoid and fully naphthalenoid [5,29,32]. Both these observations suggest that a toroidal polyhex, in properties dependent on π-electrons, is likely to resemble graphite more than fullerenes or benzenoids.

There are two reasons why varying ring sizes within the network on a toroidal surface might be considered. One is for engineering or mechanical reasons – to relieve the strain of curvature. The other, more hypothetical one, is to do with its electronic structure and π-bonding system, because seven membered rings present in a conjugated polycyclic structure have the potential for tropylium ion formation by the drift away of an electron to generate an aromatic sextet. This accounts for a great deal of azulene chemistry [42,43]. (Azulene is similar to naphthalene in having a 10-carbon atom periphery, but it consists of a pentagon–heptagon pair, not a double hexagon.)

Molecular mechanics calculations suggest that the number of vertices required to allow mechanical strain to approach an approximation of buckminsterfullerene levels

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[1] Note: in Vega there is a procedure that produces a number of transformations, including a leapfrog transformation on any cage (polyhedron, torusene, map on a Klein bottle, etc.).
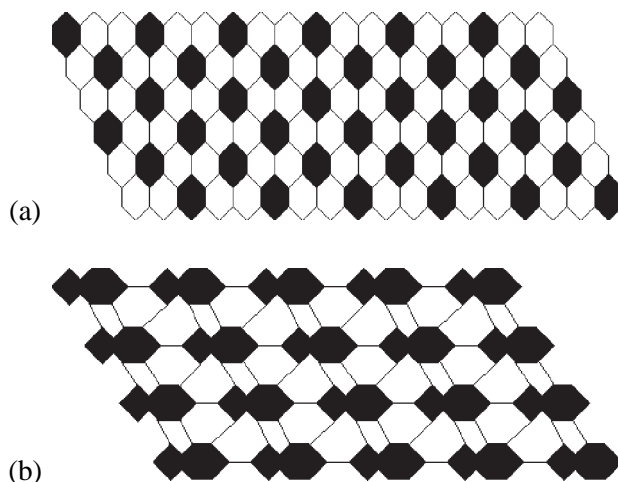
(a)

(b)

Figure 2. Two examples of fully-arenoid networks that could be put onto a torus; (a) fully benzenoid (by identifying opposite sides of the quadrilateral), and (b) fully-azulenoid (by identifying the opposite bounding rows and columns). Such structures are called fully arenoid because they *can* be represented as a set of disjoint aromatic units – in this case benzenoid or azulenoid – that account for all the atoms/vertices, and are joined by single chemical bonds. Whether this possibility has chemical significance is an open question.

can be considerably reduced by introducing seven membered rings. Euler's generalised equation requires that for a 5,6,7 ring size torus the number of five and seven membered rings must be equal. This can be satisfied by the presence of azulene units, and tori capable of being 'fully azulenoid' (figure 2(b)), provided that at least some of their azulene units remained approximately coplanar and so had some effective π-orbital overlap, could be of interest in their chemical and electrical conductance properties.

3.   Nicegraph drawings of toroidal fullerenes

Some pictures have already been published (see, for example, [47–49] besides a number of torus illustrations obtained by other means [19,21,23–26]). Figure 3 shows a typical example of (a) a toroidal polyhex (with 360 vertices), and (b) a smaller torusene having 90 vertices and five, six and seven membered rings. In the former it can be seen – and this is typical of the polyhexes – that the preferred optimal geometric drawing has a rather flattened tube, i.e., it tends to resemble a double cylinder more than the familiar 'doughnut' shape intuitively associated with the torus. Although not a necessary consequence, it inspires the thought that possibly in a real carbon structure the high energy cost of what seems unnecessarily sharp local curvature would be a worthwhile exchange for near planarity over much of the rest of the surface, so that something like this would be the most stable shape. For certain isomers, where hexagon orientations on both walls match one another, and if the tube was *very* flat,
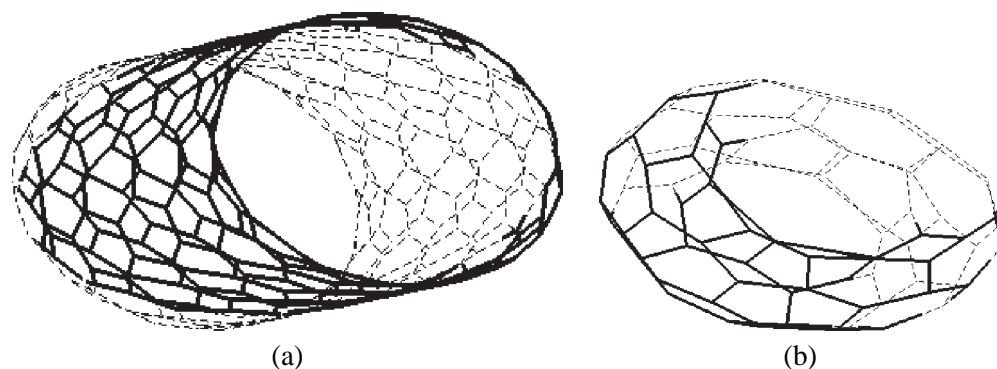
Figure 3. (a) A large (360 vertex) toroidal polyhex, and (b) a smaller (90 vertex) torusene having five, six and seven membered rings present.
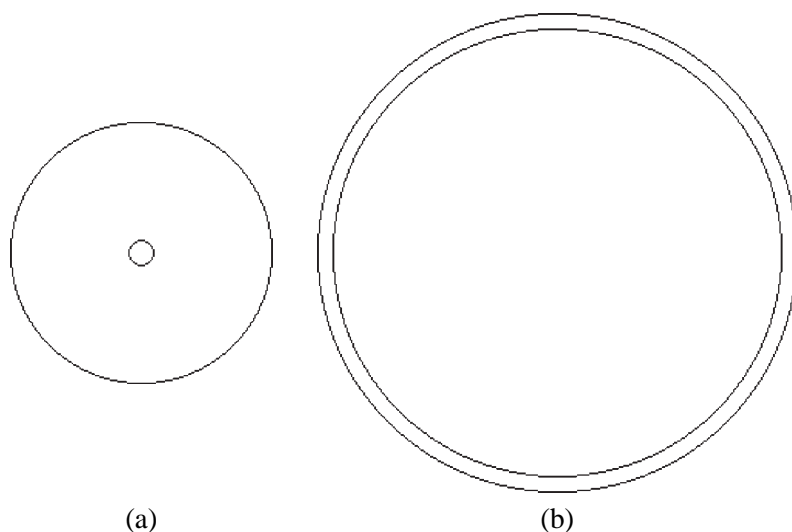

Figure 4. Toward the two extremes of strained high curvature tori.

this effect would be enhanced by weak Van der Waals bonding, of which no account is taken by these NiceGraph algorithms.

Taken to larger sizes, such structures are of course similar to tubules already known, and differ only in their capping. This would suggest that for polyhexes, a recognisably toroidal shape may only emerge with a fairly small $r : R$ ratio (figure 1), i.e., one more like figure 4(b) than figure 4(a). However, it is important at this point to remind ourselves of some of NiceGraph's limitations. It has no feeling for the 'real world'. As a variant of the so-called 'simulated annealing' method it is an iterative procedure that starts with some state and then tries to find a state with locally minimal 'energy'. In this process it can violate all kinds of physical or chemical rules. So, for example, an atom may pass through another one, and (especially relevant to these 'cage' structures) it does not know that one edge or bond cannot pass through another.

It will not recognise any entrapment of a smaller cage within a larger one unless it is held in place by bonds. There is also no chemical expertise involved concerning what angles, dihedral angles and bond lengths are plausible, and no distinction between single and multiple bonds.

4.   Torus radii proportions

Quite apart from the conclusion of the preceding section, we know that for a given size (number of vertices for a network; surface area of a continuous skin) of torus, a minimum formation energy cost must lie somewhere between the tori formed from the 'shortest fattest' possible cylinder (figure 4(a)) and the 'tallest thinnest' one (figure 4(b)). The surface area of a torus is the same as that of a cylinder, but conversion of a cylinder into a torus results in a redistribution of area about a nodal radius. In figure 1, the surface within radius R is compressed, while outside it the surface is stretched. In the case of bending a solid skin (metal or glass, say), then, roughly speaking, either the 'surface' suffers catastrophic buckling (figure 5) or it rearranges itself to a smoothly curved shape. In the latter case, *either* the material will anneal (if malleable enough or of the right viscosity) *or* it will have locked-in potential energy of stress. The position of a cylindrical *network* undergoing this process is similar, but with the added complication that strain can also be alleviated by local distortion of ring shapes and bond angles. (For example, a hexagon lying on the shorter (inner) perimeter may assume a boat conformation in order to reduce its effective length.) If a toroidal ring system is mapped onto a doubly periodic planar pattern, it will usually be the case that more than one parallelogram may be chosen to define the pattern and hence the structure (see figure 6). To these we can ascribe lengths and breadths in topological units (hexagon widths in the case of a toroidal polyhex). Intuitively we expect the range of these parallelograms to place some constraints upon any realised
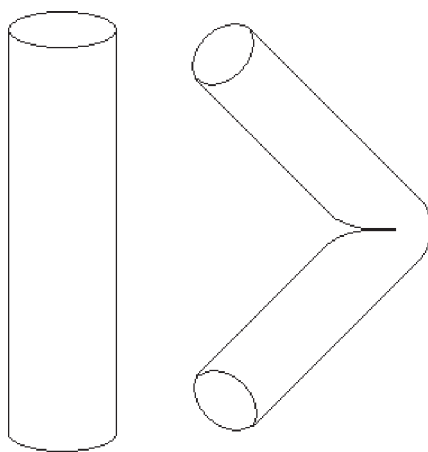

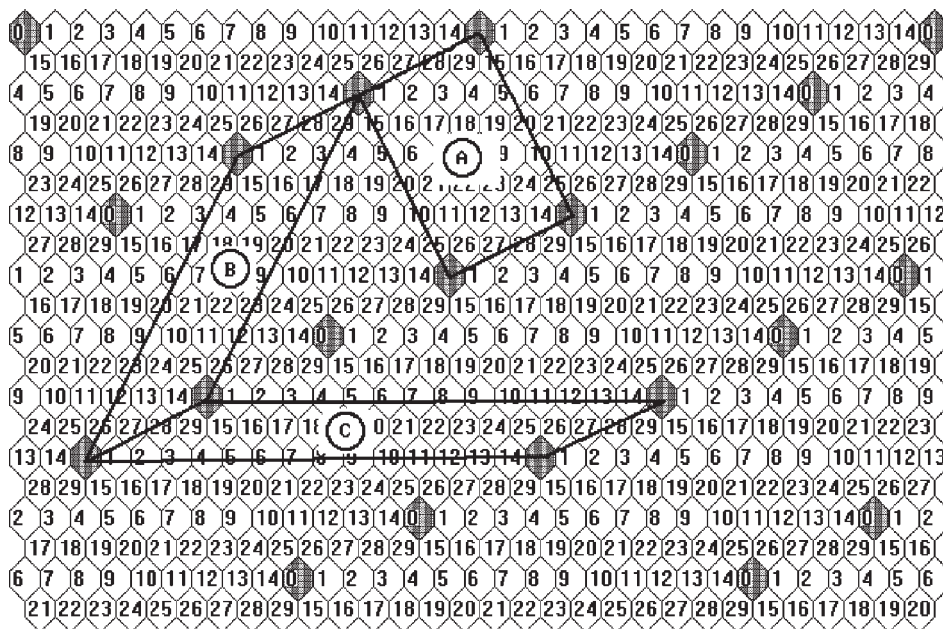Figure 5. A cylinder and its possible catastrophic accommodation to the stress of bending.

Figure 6. A planar representation of the C_{60} toroidal polyhex with canonical code 15-5-2 (see [34] for details), for which there are three sizes of quadrilateral that could be used to define it: $A = 5 \times 6$, $B = 10 \times 3$ and $C = 15 \times 2$ hexagons. How far, if at all, do these relate to the geometric ratios of a real toroidal realisation?

Table 1
C_{60} toroidal polyhexes: equivalent 'graphite quadrilaterals' available, and the size of tube shown by the NiceGraph model. (The 13 isomers are given in the order shown in figure 7.)

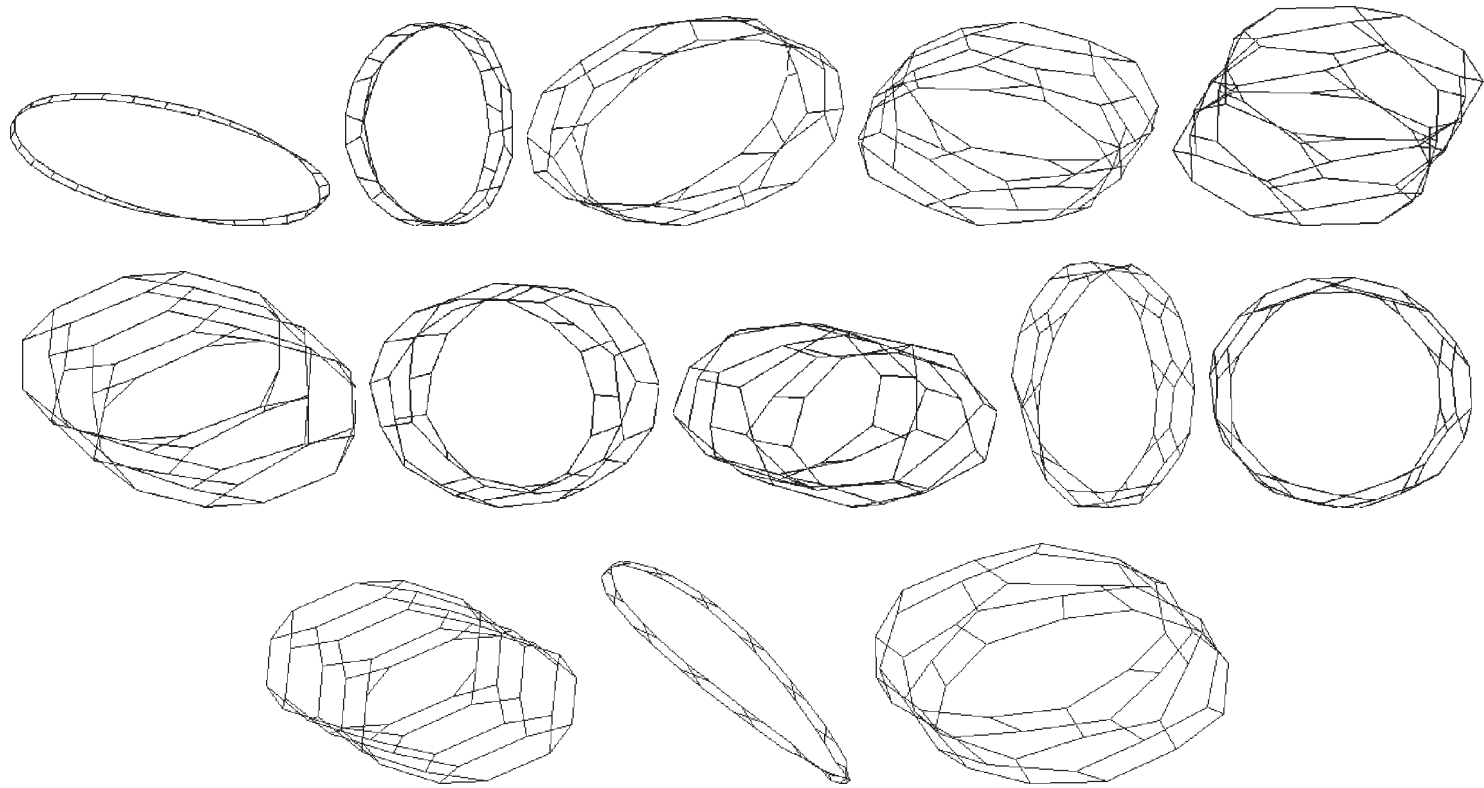|	Possible topological sizes of quadrilateral (unit size one hexagon)				Smallest edge cut through tube in NiceGraph model (unit size one connection)
	30×1 :	15×2 :	10×3 :	6×5	
1	*	*			2
2	*	*	*		3
3	*	*	*		4
4	*	*		*	5
5	*			*	5
6	*			*	5
7	*	*			4
8	*	*	*		6
9	*		*		3
10	*		*		3
11	*			*	5
12	*	*			2
13		*	*	*	5

Figure 7. NiceGraph drawings of the 13 C_{60} toroidal polyhexes. The last one is TPH(15-5-2) whose planar diagram is shown in figure 7. (Note that the first one is only formally a toroidal polyhex, in the sense that it *can* be formulated as such, but is more familiar as a (planar) cyclic ladder or even-sided prism.)

geometry, but within these and their plausible geometric distortions, which will actually be chosen? If pressed to make a wild guess, one might suspect it to involve the well-known "Golden Ratio", but we do not know and this is still an open question. Figure 7 shows NiceGraph drawings of the 13 C_{60} toroidal polyhexes. It is, in fact, not very easy to count with certainty the relative dimensions in terms of hexagons or vertices, even for these comparatively small systems. What *can* be seen and measured reliably is the minimum cut size of the tube, i.e., the minimum number of edges which need to be cut to sever the tube and turn it back into a cylinder. Table 1 shows these numbers together with the topological dimensions of available polyhex quadrilaterals. Evidently, there is a broad but imperfect correlation between the two, with a tendency (but only a loose one) for the structure to 'choose' a more nearly square possibility when it is there. Fowler and Yoshida [11] recently plotted QCFF energies against the topological length/breadth ratio, and concluded that from a high energy square form, the energy drops and reaches a more or less constant level at a ratio of around 3 to 4 (and, in passing, we might note that $3 < 2 \times$ Golden Ratio < 4). Examination of the pictures of equilibrium structures computed by these authors showed that although superficially showing some differences of shape, the edge cut number of each tube was the same as reported here for NiceGraph. Finally, before leaving tori, attention is drawn to a recent paper with the intriguing title *Fullerene crop circles* [41]. It seems that toroidal carbon is a physical reality under the right conditions.

5. Klein bottle fullerenes

As with a torus, a Klein bottle can be made by bending round a cylinder and joining the two ends, but in this case, instead of bringing the two ends 'face to face' they are joined 'face behind face', as shown in figure 8.

Like the torus it can, at least mathematically, be tessellated entirely with hexagons, but unlike the torus it has only one, non-orientable, side of a surface, which intersects with itself in 3D space. This self-intersection could in theory be implemented in a number of ways in the physical world, for example:

1. By letting the network form catenane-style links with itself, so that a cylindrical set of bonds in one part of the network passes through rings situated in another part, and there is no physical contact in the plane of surface intersection. This is the 'mathematically pure' method, which preserves the possibility of all-hexagon tessellation, but real atomic sizes and bond lengths render it implausible for 3-valent carbon structures. However, one cannot rule out the possibility that some other kind of chemical network might be realisable in this form. It is therefore of some interest to test NiceGraph models. Typically, it is not immediately obvious from the drawing produced that it is not a torus, for the NiceGraph algorithm does not care about preserving a non-crossing embedding; rather it simply forces the structure into the nearest overall shape it can get to a torus. Viewed globally, from most directions this kind of torus and its corresponding Klein bottle are hard to
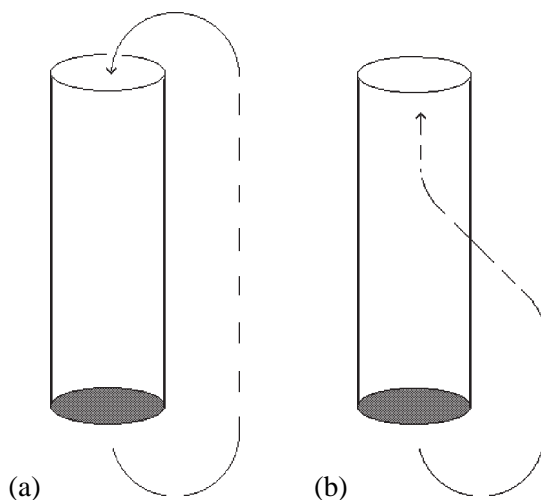
Figure 8. Conversion of a cylinder into (a) a torus by joining the ends 'face to face', and (b) a Klein bottle by joining them 'face behind face'.
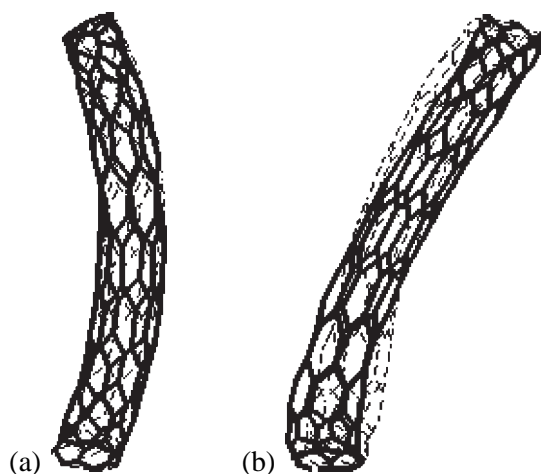

Figure 9. NiceGraph models of (a) a torus, and (b) a Klein bottle of the same size. NiceGraph ignores any attempt to preserve a locally planar embedding, and instead forces a near-toroidal global geometry. Since in large systems it becomes difficult to track individual connections, the only *easy* way the difference here may be discerned is when the objects are viewed sideways, for this Klein bottle betrays itself with a global twist that cannot be hidden.

tell apart. A clear difference can, however, be seen when they are viewed together 'edgewise', as in figure 9.

2. By creating a surface intersection line where edges from its vertices go in sequence to each of the four incident network surfaces. This method creates a continuous polycyclic network over the entire surface, albeit not one of uniform density and ring size. We have not pursued this method any further. It can be questioned
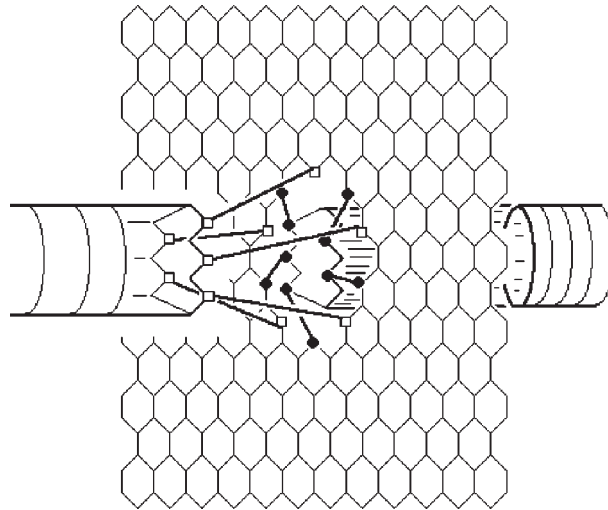
Figure 10. Construction of a Klein bottle with connections where the surface self-intersects. Here the tail of a large cylinder has been tapered down to a circumference of five hexagons and is attached to a hole with ten 2-valent vertices made in the polyhex cylinder wall, and another cylinder section joined the other side. The result is a polyhex cylinder that passes through a polyhex sheet, although it cannot preserve an all-hexagon formulation at the join (and in any case, a polyhex cylinder cannot be tapered and remain a polyhex).

whether this (or case 3 below) should be called a Klein bottle in strict topological terms, but here we categorise it loosely as such for convenience. Strictly speaking the result of this process is not a surface anymore. By definition, a surface is locally a plane, and a surface cannot be distinguished from a plane for points within a small neighbourhood. In case 2 (or 3) there are actually "singular points" on the self-intersection which have non-planar neighbourhoods. (A singular point is locally like a point on a spine of a book with 4 leaves (8 pages).)

3. This is a simpler version of the last method: A 'hole' of degree-two vertices is made in one part of the surface, of a size corresponding to twice the circumference (in free 2-valent vertices) of the tapered cylinder end, and then two sections of the narrower tube are joined to this by alternate edges (figure 10). The result is a hollow tube passing through and joined to the larger surface wall. However, when a complete Klein bottle is constructed by this method, the NiceGraph algorithm refuses to display it properly because it will not accept the internal (and thinner) section of the tube; preferring instead to force it outside the 'bottle' to form a near-double-torus (figure 11).

For most tori, the eigenvectors of the 2nd, 3rd and 4th largest eigenvalues of an adjacency matrix yield a drawing which usually makes apparent the toroidal topology, although it does not always show a clear distinction between a torus and a cycle or cylinder. Conversely, from a drawing alone, one cannot be sure that what appears to be a cycle or cylinder may not, in fact, be a torus. The NiceGraph Spring Embedder
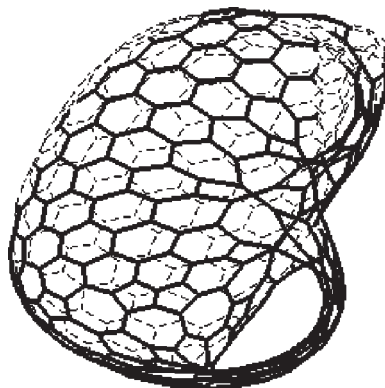
Figure 11. A completed Klein bottle using the connection type shown in figure 10. This resembles a near-double-torus. A planar embedding is not preserved because NiceGraph will not tolerate the internal section of the tapered cylinder.
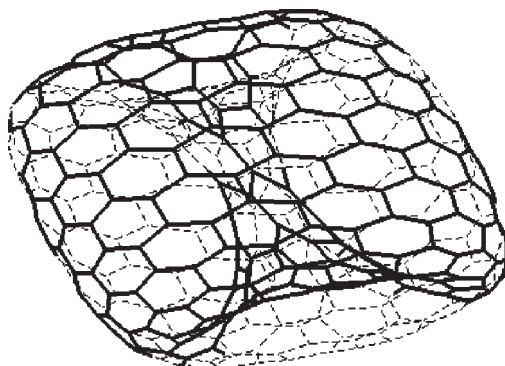

Figure 12. A torus made by joining the two ends of a tapered cylinder; but if the narrow section is made any longer than shown here, NiceGraph will force it outside the larger section (figure 13).

routines, on the other hand, always give a reasonable, even if rather flattened, drawing of a torus with a tube of uniform diameter.

Where the tube size is not uniform, however, other complications can arise, and these are pertinent to the behaviour of Klein bottles described above. For example, figure 12 shows a 'fat' torus made by joining a relatively narrow tube inside a relatively fat (almost spherical) tapered cylinder. Under NiceGraph, a drawing of this type is very sensitive to the relative topological dimensions, for if the length of the inner – in relation to the outer – tube only slightly exceeds that shown, it will be pushed outside with resultant twisting into what appears to be a Klein bottle form (figure 13(a)).

Similarly, as was mentioned earlier, all attempts so far to construct a conventional looking Klein bottle have resulted in non-cage-like but near-toroidal structures. This effect can be seen in a simplified context in figures 14 and 15, which show that a cylinder passing through a large polyhex sheet as shown in figure 10 cannot be modelled by this method – because both cylinders are forced to one side, by repulsion

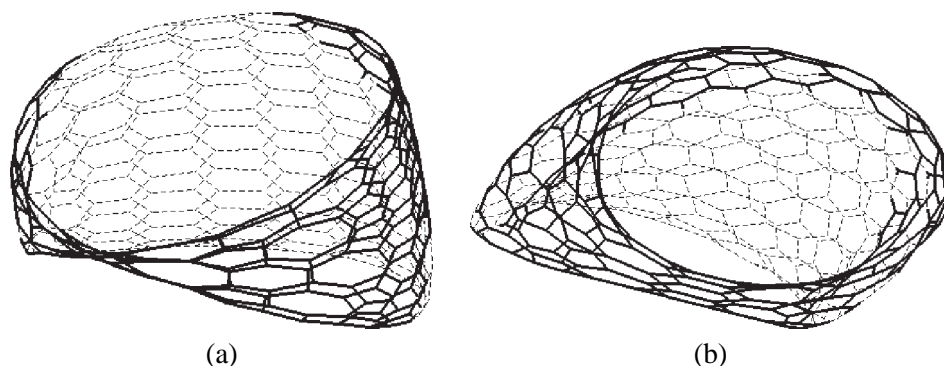(a)   (b)

Figure 13. The result of joining a slightly longer version of the cylinder used for figure 12. In (a) the narrow tube has been forced outside to give an apparently Klein bottle topology; in (b) the same is reconnected to give a true torus.

from the sheet. In consequence, however, this affords a method for making a slightly more realistic version of a Klein bottle of the self-linked type 1 described above, by giving the bottle a large lip (see figure 16).

6.   Other kinds of isomerism and other kinds of topology

There is of course a whole universe of possible cage-like structures, of which only a few, so far, have been conceived of. Even for the simple torus there are possible modes of stereoisomerism (i.e., beyond connectional isomorphism) which have been ignored here. We have touched upon the uncertainties in our knowledge of the dimensional proportions that would be chosen by a physical toroidal network. Some alternatives are likely to be distinct geometric isomers; others not. Some toroidal networks with more than one face size will be chiral. There will be at least the *possibility* (even if energetically they are unlikely) of 'super-twisted' isomers. These may be imagined as tori made from cylinders that, before joining, have been twisted so far that the cyclic permutation of possible connections has already gone through more that one cycle before these connections are actually made. Going further, and necessarily requiring larger structures with more atoms or vertices, combinations of toroidal rings can be imagined. Figure 17 shows one example of a double torus (this one has 340 vertices). In the family of double tori, besides the greatly increased number of 'twisting' isomers within each tube, the whole can be formulated to have different orientations of the two rings with respect to each other. There is a simpler version of this (in terms of connectivity): two tori with a catenane type of linking (figure 18).

Here we have two levels of genus; the non-planar linking of two non-planar genus-one objects. Having done that, why should we not take a single very long carbon cylinder and tie knots in it before joining to a torus? And so on . . . Obviously, these are more complicated objects. If one considers physical 3D realisations of closed surfaces
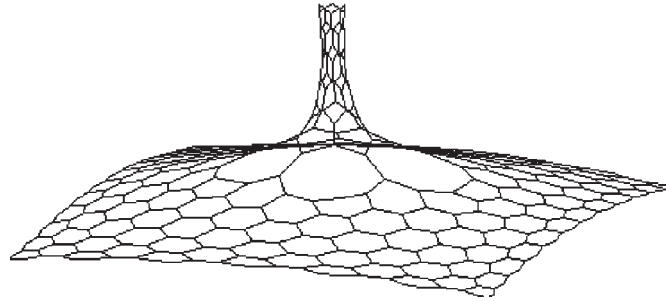
Figure 14. One cylinder of five hexagon circumference joined to a hole in an open polyhex sheet (cf. figure 10).
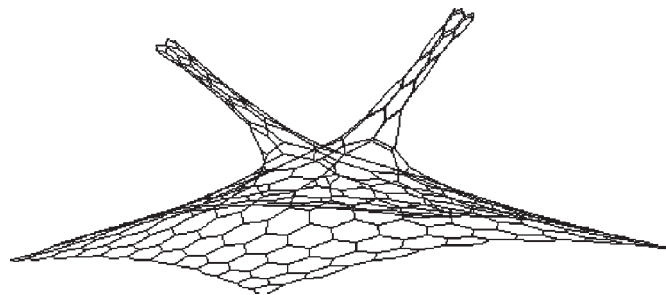

Figure 15. A continuation of figure 14 (cf. figure 10) in an attempt to reproduce the intended process shown in figure 10 of passing a cylinder through a polyhex wall with connections at the intersection. Even here, with an open finite polyhex sheet, NiceGraph forces both cylinders to one side and does not allow the intended embedding.
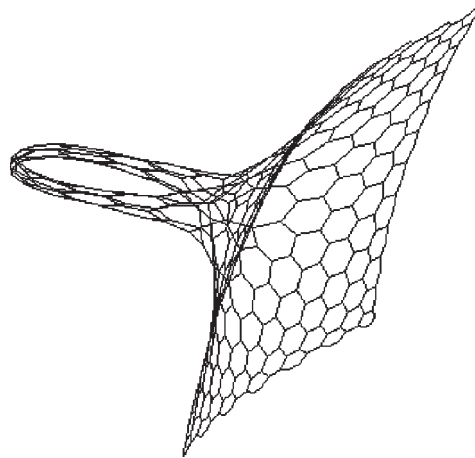

Figure 16. Although difficult to see in a static mode, the behaviour of NiceGraph *does* allow another kind of Klein bottle to be formulated. Here a polyhex cylinder is brought round for 'face behind face' joining, but is stitched alternately to the rim of the hole in a polyhex sheet which serves to stabilise the configuration.
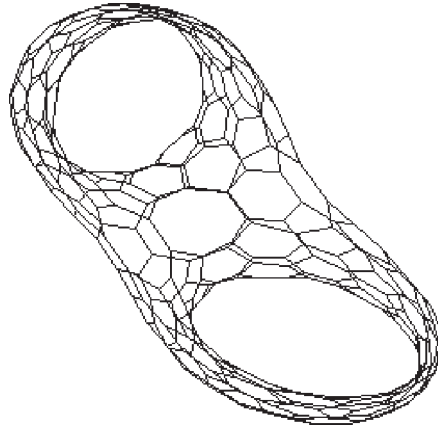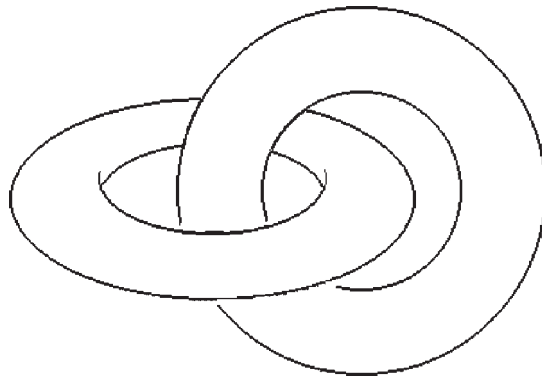
Figure 17. A 340-vertex double torus.

Figure 18. A catenane-linked type of double torus.

(compact surfaces without a boundary) then all *orientable* surfaces admit realisation without self-intersections. In particular, this is true for the sphere, torus, double torus, triple torus, etc. For an ordinary torus, there is a more or less standard representation, and the still open question is – what is its best radius ratio $r : R$?

On the other hand, each 3D realisation of any *non-orientable* closed surface (projective plane, Klein bottle, etc.) must contain self-intersections. If a boundary is allowed then this problem can be side-stepped: for instance, the Möbius band can be placed in 3D space without self-intersection. But whenever a disk is glued onto its boundary to make it a projective plane, the self-intersections are bound to occur.

Reverting to the torus, what the 'standard' 3D representation of the double torus should be is an interesting but rather more difficult question. Is it a sphere with two handles? Is it a pretzel? Or is it three parallel tubes that are curved at both ends and glued together? The latter representation is the most symmetric. It has a dihedral symmetry. The abstract group has 6 elements, and so it may be considered standard. It is interesting that NiceGraph tends to present such a representation in several cases.

We are working to try to find the 'most symmetric' representation of other surfaces, such as triple torus, quadruple torus or projective plane, Klein bottle, etc.

The familiar representation of the Klein bottle lacks symmetry, and is perhaps one plausible explanation of why it is so difficult to model it with our programs.

Acknowledgements

References

[1] J.E. Avron and J. Berger, Phys. Rev. A 51 (1995) 1146–1149.
[2] J. Berger and J.E. Avron, J. Chem. Soc. Faraday Trans. 91 (1995) 4037–4045.
[3] B. Borštnik and D. Lukman, Chem. Phys. Lett. 228 (1994) 312–316.
[4] G. Brinkmann and A.W.M. Dress, Preprint (1996).
[5] J. Brunvoll, B.N. Cyvin, S.J. Cyvin, E.C. Kirby and I. Gutman, Polycyclic Aromat. Comp. 4 (1995) 219–229.
[6] A. Ceulemans and P.W. Fowler, J. Chem. Soc. Faraday Trans. 91 (1995) 3089–3093.
[7] B.I. Dunlap, Phys. Rev. B 46 (1992) 1933.
[8] P. Eades, Congr. Numer. 42 (1984) 149.
[9] P. Fowler and T. Pisanski, J. Chem. Soc. Faraday Trans. 90 (1994) 2865–2871.
[10] P.W. Fowler, T. Pisanski and J. Shawe-Taylor, in: *Graph Drawing*, eds. R. Tamassia and I.G. Tollis, Lecture Notes in Comput. Sci., Vol. 894 (Springer, Berlin, 1995) pp. 282–285.
[11] P.W. Fowler and M. Yoshida, Personal communication (1996).
[12] T. Fruchterman and E. Reingold, Software Pract. Exp. 21 (1991) 1129–1164.
[13] C.D. Godsil, *Algebraic Combinatorics* (Chapman and Hall, 1993).
[14] J.C. Greer, S. Itoh and S. Ihara, Chem. Phys. Lett. 222 (1994) 621–625.
[15] C.W. Haigh, Personal communication (2 March 1995).
[16] H. Hosoya, Y. Okuma, Y. Tsukano and K. Nakada, J. Chem. Inf. Comput. Sci. 35 (1995) 351–356.
[17] H. Hosoya and Y. Tsukano, *2-Dimensional Torus Benzenoids whose Electronic State Rapidly Converges to Graphite* (Victoria, BC, 1992).
[18] H. Hosoya, Y. Tsukano, M. Ohuchi and K. Nakada, Two-dimensional torus benzenoids whose electronic state rapidly converges to graphite, Fac. Sci., Ochanomizu University, Tokyo (1993).
[19] S. Ihara and S. Itoh, Phys. Rev. B 47 (1993) 12 908–12 911.
[20] S. Ihara and S. Itoh, Carbon 33 (1995) 931–939.
[21] S. Ihara and S. Itoh, Surface Rev. Lett. 3 (1996) 827–834.
[22] S. Itoh and S. Ihara, Phys. Rev. B 48 (1993) 8323–8328.
[23] S. Itoh and S. Ihara, Phys. Rev. B 47 (1993) 1703–1704.
[24] S. Itoh and S. Ihara, Phys. Rev. B Condens. Matter 49 (1994) 13 970–13 974.
[25] P.E. John and B. Walther, Mögliche Strukturen und Linearfaktoranzahlen Toroidaler Hexagonaler Systeme, Technische Universität Ilmenau (1993).
[26] P.E. John and B. Walther, Sketch about possible structures and numbers of perfect matchings of toroidal hexagonal systems, Fakultät für Mathematik und Naturwissenschaften, Technische Universität Ilmenau (1994).
[27] J.K. Johnson, B.N. Davidson, M.R. Pederson and J.Q. Broughton, Phys. Rev. B Condens. Matter 50 (1994) 17 575–17 582.
[28] T. Kamada and S. Kawai, Inf. Process. Lett. 31 (1989) 7.

[29] E.C. Kirby, Croat. Chem. Acta 66 (1993) 13–26.

[30] E.C. Kirby, Fullerene Sci. Technol. 2 (1994) 395–404.

[31] E.C. Kirby, Croat. Chem. Acta 68 (1995) 269–282.

[32] E.C. Kirby, MATCH 33 (1996) 147–156.

[33] E.C. Kirby, in: *From Chemical Topology to Three-Dimensional Geometry*, ed. A.T. Balaban (Plenum-Press, New York, 1997) pp. 263–296.

[34] E.C. Kirby, R.B. Mallion and P. Pollak, J. Chem. Soc. Faraday Trans. 89 (1993) 1945–1953.

[35] E.C. Kirby, R.B. Mallion and P. Pollak, Mol. Phys. 83 (1994) 599–602.

[36] E.C. Kirby and P. Pollak, J. Chem. Inf. Comput. Sci., in press.

[37] D.J. Klein, J. Chem. Inf. Comput. Sci. 34 (1994) 453–459.

[38] D.J. Klein and X. Liu, Int. J. Quantum Chem. 28(Suppl.) (1994) 501–523.

[39] D.J. Klein and H. Zhu, Personal communication (1994).

[40] D.J. Klein and H.Y. Zhu, in: *From Chemical Topology to Three-Dimensional Geometry*, ed. A.T. Balaban (Plenum-Press, New York, 1997) pp. 297–341.

[41] J. Liu, H.J. Dai, J.H. Hafner, D.T. Colbert, R.E. Smalley, S.J. Tans and C. Dekker, Nature 385 (1997) 780–781.

[42] D. Lloyd, *Non-Benzenoid Conjugated Carbocyclic Compounds* (Elsevier, New York, 1984).

[43] D. Lloyd, J. Chem. Inf. Comput. Sci. 36 (1996) 442–447.

[44] D.E. Manolopoulos and P.W. Fowler, J. Chem. Phys. 96 (1992) 7603.

[45] D.E. Manolopoulos, D.R. Woodall and P.W. Fowler, J. Chem. Soc. Faraday Trans. 88 (1992) 2427–2435.

[46] T. Pisanski, *Vega 0.2 Quick Reference Manual and Vega Graph Gallery* (Ljubljana, 1995); also at http://vega:ijp.si/.

[47] T. Pisanski, M. Kaufman, D. Bokal, E.C. Kirby and A. Graovac, J. Chem. Inf. Comput. Sci. 37 (1997) 1028–1032.

[48] T. Pisanski, B. Plestenjak and A. Graovac, Croat. Chem. Acta 68 (1995) 283–292.

[49] T. Pisanski and J. Shawe-Taylor, Preprint (1994).

[50] M. Randić, Y. Tsukano and H. Hosoya, Natural Sci. Rep. Ochanomizu Univ. 45 (1994) 101–119.

[51] H. Sachs, J. Chem. Inf. Comput. Sci. 34 (1994) 432–435.

[52] H. Sachs, P. Hansen and M. Zheng, Personal communication (1994).

[53] H. Sachs and P. John, Personal communication (1994).

[54] T.G. Schmalz, W.A. Seitz, D.J. Klein and G.E. Hite, J. Am. Chem. Soc. 110 (1988) 1113–1127.

[55] J. Shawe-Taylor and T. Pisanski, Characterising graph drawing with eigenvectors, Department of Compuer Science, University of London (1994).

[56] C. Thomassen, Trans. Amer. Math. Soc. 323 (1991) 605–635.

[57] R. Tosić and S.J. Cyvin, Zb. Rad. Prirod.-Mat. Fak. 22 (1992).

[58] M. Yoshida, M. Fujita, P.W. Fowler and E.C. Kirby, J. Chem. Soc. Faraday Trans. 93 (1997) 1037–1043.