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Remarks Upon Recognising Genus and Possible Shapes of Chemical Cages in the Form of Polyhedra, Tori and Klein Bottles

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Some of the problems associated with recognising and classifying cage structures are reviewed briefly and discussed. Some new structures are considered, including Klein bottles (polyhex and azulenoid) and 'near polyhex' double tori.

1. INTRODUCTION

Since the discovery of buckminsterfullerene, great interest has attached to the general concept of molecules that consist of a boundless two-dimensional lattice enclosing a portion of 3D-space (cages). Good evidence has been amassed for the existence of spherical and cylindrical structures made of networks with five and six-membered rings. The theoretical possibility of toroidal forms of benzenoids, azulenoids and others has been pointed out,[1–5] but no fully comprehensive taxonomy of all possible forms of cage structure seems to have been attempted, nor is it achieved here. The problem (which is really a cluster of problems) is difficult, for reasons that are discussed below.

Our studies have been restricted to graphs consisting of a set of vertices in which every vertex is adjacent to three others. In other words to trivalent or cubic graphs, which of course can represent all-carbon molecules in which the carbon atom's four (sigma) bonds are hybridized to three π-bonds tending to seek a planar 120° disposition. The problem may be expressed in the form – »given a molecular cluster of n 3-valent carbon atoms (equivalent to a cubic graph) generated at random, how can one know all the possible cage structures which could be assumed, ignoring at this stage any suspected chemical constraints?«

Even with this limitation to regular graphs of degree 3 the subject is not an easy one, for reasons that include –

1) Combinatorial complexity; as the number of vertices increases, so too does the number of possible arrangements, typically at an ever increasing rate; a problem common to most molecular enumerations.

2) Lack of useful graph invariants; only very limited help is available from currently known theorems in graph theory.
3) The isomorphism problem; when classifying structures there is frequently the need to decide whether two apparently quite different structures are in fact the same. This is well known to be difficult, although it *seems* to have been largely solved for this group.[6]
4) Recognition difficulties. These are related to 3) above, but are wider in scope. The act of recognising whether two graphs are the same or whether they are even related in some way (by being of the same genus, or by having some common subgraph, for example), is difficult, whether attempted directly and intuitively, or *via* an efficient computer algorithm. So also is the converse problem – seeking alternative forms of interest that a given graph might display.

Accordingly, the subject is best considered from two directions; (i) by checking and applying whatever fundamental principles are available and appropriate, and (ii) by formulating specific structures, and noting their properties, so that these at least may be recognised when they are found among other, strange ones.

There is of course a third approach; that of determining optimum geometries on a heuristic basis by considering the energetic strains in a molecule by molecular mechanics, but, important as this necessary process is, and complementary to this discussion, it is not considered further here.

2. GENERAL PRINCIPLES AND DEFINITIONS

2.0 In general, Wilson's conventions of graph theory[7] are followed.

2.1 THE CONNECTIVITY OF A GRAPH

This is the smallest number of vertices whose removal disconnects the graph. There is an analogous version applying to edges. For the present discussion, structures with a vertex connectivity of less than three are regarded with little interest, because – intuitively speaking – they do not lend themselves to forming simple 'all-enclosing' network cages. It is easy to write a reliable computer algorithm for determining this.

2.2 THE GENUS OF A SURFACE

A rigorous definition of the genus of a surface is best sought from mathematical textbooks (see references cited by Devlin[8] for example), but loosely speaking it refers to the number of holes it has. So an infinite plane, or the surface of any 'solid' object like a polyhedron or sphere is of genus-zero, whereas a torus has a genus of one, and an object of genus-two would have two holes in it (for example, a two-handled coffee cup). A planar or zero-genus surface can be distinguished from others by the fact that *any* circle on it, wherever it is placed, can be contracted to a point without cutting or leaving the surface.

2.3 THE GENUS OF A GRAPH

This is the genus of the lowest genus surface on which the graph can be drawn without crossing (*i.e.* embedded). It is well known (Kuratowski's Theorem[7]) that a necessary and sufficient condition for a graph to be planar (of zero-genus) is that it does not contain either K_5 or $K_{3,3}$, or any subdivision (see 2.4) of either, as a subgraph. This theorem is useful when, often by chance, such subgraphs are recognised, but devising a reliable means of recognition has proved to be too difficult to make this method generally useful.

There are some efficient practical algorithms available for testing planarity, *i.e.* for testing whether or not $g = 0$, based on systematic techniques for constructing planar drawings. Workers include Goldstein,[9] Fisher and Wing,[16] Booth and Leuker,[11] and Hopcroft and Tarjan;[13] see Refs. 13 and 14 for useful reviews of these and other papers on planarity testing.

2.4 A SUBDIVISION OF A GRAPH

A subdivision of a graph is one that has been enlarged by the insertion of one or more degree-2 vertices into its edges. The extent and pattern of branching (and hence whether or not it is planar) is unaffected.

2.5 THE COUNT OF SMALLEST CIRCUITS

Here this phrase is used to refer to the total number of the smallest ring or circuit present, followed by the total numbers of each increasing ring size, carried to an arbitrary extent depending on requirements.

2.6 THE EULER AND OTHER RELEVANT FUNDAMENTAL RELATIONSHIPS

For a graph with n vertices, m edges and f faces, with g being the genus, and v_i the degree of any vertex i, the generalised Euler relationship gives

$$n - m + f = 2 - 2g \tag{1}$$

The general handshaking lemma gives

$$\sum_{i=1}^{n} v_{\mathrm{i}} = 2m \tag{2}$$

and so, for a cubic graph

$$\mathrm{m} = 3n/2\ . \tag{3}$$

It follows that in general

$$\mathrm{f} = n/2 + 2 - 2g, \tag{4}$$

and in particular

$$\mathrm{f}_{\mathrm{planar}} = n/2 + 2, \tag{5}$$

$$\mathrm{f}_{\mathrm{toroidal}} = n/2\ . \tag{6}$$

If we stipulate that for a cage representation every vertex should be shared by three faces, then

$$\Sigma \text{ (face size)} = 3n \ . \tag{7}$$

Every face must be a circuit in the graph. It therefore follows that we can state two bounding conditions:

1) There must be a set of smallest circuits where Σ (circuit size) $\leq 3n$,

2) There must be a set of largest circuits where Σ (circuit size) $\geq 3n$

The first condition is the more useful one in practice.

2.7 POLYHEDRAL CAGE

This is taken to be a boundless network that can be embedded on a spherical, or – by Schlegel projection – on a planar surface. It is 3-connected, and on the surface of a polyhedron every vertex is shared by three faces.

2.8 TOROIDAL CAGE

This is a boundless network that can be embedded on the surface of a torus. It, similarly, is 3-connected, and every vertex is shared by three faces. It is important to note that this definition makes no reference to genus, which, although usually of value one, may be either zero or one, and if zero capable of representation as either a polyhedral or a toroidal cage. Furthermore, a given toroidal representation is not necessarily unique; more than one set of faces may satisfy the requirements of a toroidal representation.[3,4]

It was mentioned above that 2-connected graphs are not regarded as polyhedral cages. In the context of tori, this stipulation is still valid, but is probably inadequate; toroidal polyhexes in which the torus is cut by cutting two edges (resulting in a non-toroidal but still connected graph) are toroidal and are 3-connected, but it is debatable whether they should be called *cages*, although they are not distinguished further here.

2.9 KLEIN BOTTLE CAGE

This is defined in the same manner as for the polyhedral or toroidal cages above, but using a Klein bottle (Figure 1) as the object for tessellation. Because, in 3D space, a Klein bottle has a self-interecting surface, it is necessary to explain this. Here we take it to mean that the network 'passes through' itself with a series of links involv-

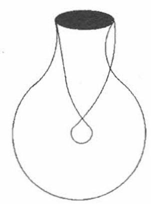


Figure 1. A Klein bottle, drawn so as to illustrate its relationship to a torus; it is a cylinder joined 'end face-behind-end face' instead of 'end face-to-end face' (*cf.* Figure 6).

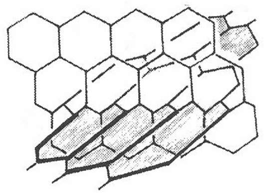


Figure 2. Two lattices intersecting without physical contact.

ing an edge passing through a face (Figure 2.). This results in a constrained, ring interlocked structure, but one that has no connectional join. An alternative treatment is to establish edge connections between the intersecting networks as shown in Figure 3.

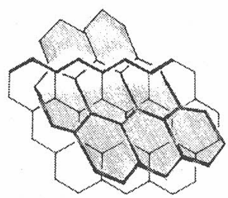


Figure 3. Two networks intersecting with a physical connection. Note that this involves non hexagonal rings at the intersection.

The choice is a matter of how the 'surface' of a network is defined. There are merits and demerits to either choice. A non-connected but interlinked intersection allows a Klein bottle with a uniform tessellation to be constructed, but for small rings, such as hexagons made of carbon, this is chemically unrealistic. On the other hand connecting the surfaces means that the connection boundary has rings that (i) are larger than elsewhere on the surface (so that the structure is not strictly a polyhex), and (ii) must, for any reasonable sized structure, have pronounced out-of-the-plane connections.

3. DISCUSSION

3.1 CLASSIFICATION

Figure 4 shows the beginnings of a classification of cubic graph types (with some examples). It is important to emphasize that what is being considered here are *representations* of cubic graphs, not just the structures themselves, so that the scheme shown does not necessarily provide a unique classification position for any given graph. Thus in Figure 4 the 'cube' graph is used as an example to illustrate both polyhedral and toroidal shapes of 3-connected genus 0 graphs, and many others can have alternative representations, while a genus 1 graph may have more than one toroi-

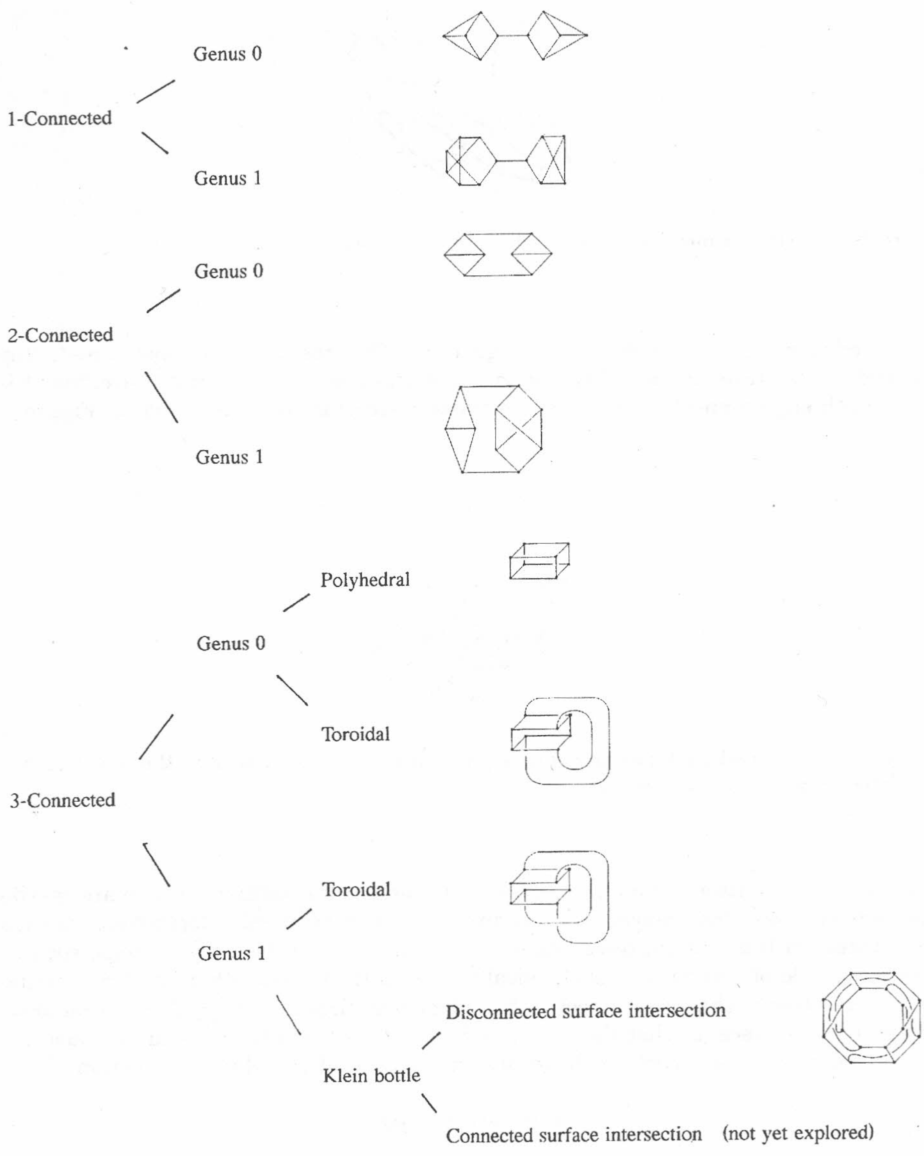


Figure 4. A partical classification of some cubic graps in relation to 'shape'

dal form and/or Klein bottle forms, depending on the number and size of circuits that are available as possible faces for an embedding. The Klein bottle example shown is a Klein bottle polyhex, but it can also be arranged or perceived as a non-polyhex toroidal graph. (It *may* be the case[15] that every Klein bottle graph has one or more isomorphic toroidal forms; we do not know).

3.2 GRAPH INVARIANTS FOR DISTIGUISHING NON ISOMORPHIC GRAPHS

The best method currently available for indexing a particular graph appears to be the combination of its eigenspectrum and its '$\boldsymbol{T}$(G)' matrix , as used previously[16] following work by Liu and Klein.[6] The conjecture that this method resolves all chemically interesting graphs appears empirically plausible, but has not been proved, so that the possibility of hidden degeneracies must be kept in mind, but no case of failure has come to light so far.

3.3. GRAPH INVARIANTS FOR DISTINGUISHING GENUS.

References to some algorithmic methods were given in 2.3 above, and it was noted that the presence or absence of subgraphs K_5, $K_{3,3}$ (or subdivisions of them) is a graph invariant that distinguishes betweeen genus = 0 and genus > 0, but it not a generally useful one.

The generalised Euler equation (2.6) is the only known simple equation giving the genus. A number of other bounds have been derived,[7] but in practice they frequently give tolerance limits that are too wide to be useful in practice, at least for this group of graphs.[15] The problem with using the Euler equation itself is that, besides the numbers of vertices and edges (unambiguous and easily measured), it requires knowledge of how many faces there are, and this is much more problematic, for it involves choosing a *suitable* set from what may be a large total number of circuits in the graph.

Generally speaking, 'genus' seems to have rather little effect upon other easily observed characteristics of graph. One interesting observation made recently,[17] is the relationship betweem the numbers of spanning trees in a labelled molecular graph and in its dual. For planar graphs they are equal, and, since the (frequently smaller) inner dual may be used (with its generalised characteristic polynomial), this often provides a means for simplifying computation, but for non-planar graphs there appears to be a variable relationship. However, construction of a dual requires knowledge of the faces, and this in turn presupposes an already existing model or drawing, so that futher work is needed before it becomes clear whether this distinction can be exploited.

In the absence of any useful general methods, one is reduced to deploying ad hoc considerations, although these can sometimes be quite effective. The *count of smallest circuits* (see above) together with the Euler equation and others (1–7) are used. The following section shows an elementary example of this.

3.3.1 *An example of genus that can easily be determined: six-vertex cubic graphs*

Cubic graphs with six vertices must have nine edges. Any structure must have five faces ($n/2+2$) for a polyhedron (g = 0) and three ($n/2$) for an object of genus one.

It is found that connection tables can be constructed for only two non isomorphic possibilities, referred to as A and B:

Counts of smallest circuits in the two structures are:

	R_3	R_4	R_5	R_6
A	2	3	6	3
B	0	9	0	6

The requirement that the sum of face sizes is $3n$ (=18) can be satisfied by $2R_3 + 3R_4$, $2R_3 + 2R_6$ or $3R_6$. $2R_3 + 3R_4$ gives the five faces required by a polyhedron, and is available for A. $2R_3 + 2R_6$ (four rings) satisfy neither the five faces of a polyhedron nor the·18 vertices of a three-faced torus. $3R_6$, on the other hand, exactly matches the requirement of a torus, and is available in B, which does not have a set of five circuits summing to 18. It follows that A and B, shown below, are of genus zero and one respectively.

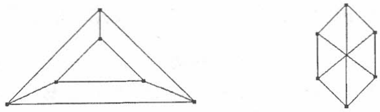


Figure 5. The two six-vertex cubic graphs.

3.2.2 *The genus of toroidal polyhexes*

Another case where elementary methods can be applied is for toroidal polyhexes.[3] These have $n/2$ hexagonal faces, and most such structures have no rings smaller than a hexagon. Since two extra faces are exhibited by a polyhedron, it is immediately obvious that no ($n/2+2$) ring set can be chosen that sums correctly to $3n$. Since by definition they *are* embeddable on a torus, their genus must be unity. These considerations narrow down the field to leave two series that do have smaller (R_4) rings, and, for these, drawings can be used to demonstrate that there is just one series of even-hexagon toroidal polyhexes that are planar rather than 'truly toroidal'. (These may also be regarded as simple cyclic ladders. They have been called 'annuluses' in recent work.[18])

Of course, the presumption that this toroidal polyhex series (referred to as TPH(h-2-1) - see Ref. 3) when h (number of hexagons) is even is the *only* planar series among *all* toroidal polyhexes, remains a conjucture.

3.4 THE CONSTRUCTION OF CAGE ADJACENCY DIAGRAMS

3.4.1 *Structures with genus ≤ 2*

As noted above, in order to complement analytical methods described so far, it is desirable to construct diagrams of cages to known specifications, and this approach has received considerable attention in the literature, especially for polyhedra,[16,19–30], but also in a few cases for other forms.[1–5,18,31–33] Balasubramanian's work[34] on enumerating substitution isomers of C_{60} should also be noted.

Among the more comprehensive and systematic studies was one made by members of the Galveston Group,[20] who introduced the term 'amenable' to describe a trivalent polyhedron with only five and six sided faces, and who counted 1790 such isomers of C_{60}, although this figure was later corrected[21] to 1812 (see also Ref. 22), classified according to two integers p and q: the number of pairs of pentagons sharing an edge, and the number of triples of pentagons sharing a vertex. (And they introduced the interesting intuitive concept of the surface being, as it were, a sea of hexagons, on which 12 pentagons float around in varying aggregates). Clearly p and q should be used as a basis for further subdivision of the category of 3-connected-zero genus polyhedra in Figure 4.

There is an important sense in which working with a toroidal surface is simpler than with a sphere. Chemists suffer the same problem as cartographers when contemplating polyhedral cages; that these can be projected onto a plane only with considerable distortion, apparently more than is the case for the torus which may more naturally be 'skinned' to give a rectangle that repeats to cover the infinite plane. (This procedure allowed the systematic three-integer code for toroidal polyhexes already mentioned to be developed, together with a method for enumeration and adjacency matrix compilation, and for deriving closed eigenvalue formulae.[3])

Another very useful method of deriving adjacency information for genus-one structures is to draw them as planar rectangles with opposite sites being made 'identical' and having the same vertex labels. This is directly analogous to manufacturing a physical torus by taking a semi-stiff rectangular sheet, and folding and gluing opposite edges, first to a cylinder and then, by joining the now-circular ends, to a hollow torus (Figure 6). If, for a given size, every shape for which this can be done is identified, and if each pair of sides (top-bottom and lef-right) is given a relative twist (a cyclic permutation from 0 up to 180 degrees) before the 'gluing' process, then all the 'connectional' isomers will be found. It should be noted that there are various other sources of possible isomerism which are not taken acount of here. These include the order in which the two 'gluings' are made; degrees of twist > 180 degrees; disconnected tori with catenane-type linking; knots tied in the torus tube, and so on. We have also arbitrarily restricted this discussion to structures where the toroidal tube is of uniform radius.

This method can be adapted for Klein bottle construction. The requirement is to join one end of the intermediate cylinder 'from behind' rather than 'face-to-face with' the opposite end. This is achieved simply by labelling the equivalent vertices in the opposite sense around one end.

Alternatively, the process may be divided into two stages. Two rectangles are drawn; each is converted to a cylinder, and the two cylinders are joined end-to-end to form the torus. If each rectangle is twisted at the first stage, the result is two Möbius bands. A Möbius band has only one edge (in the global not graph-theoretical sense), and if two are joined, the result is a Klein bottle (Figure 7).

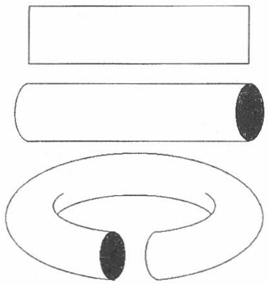
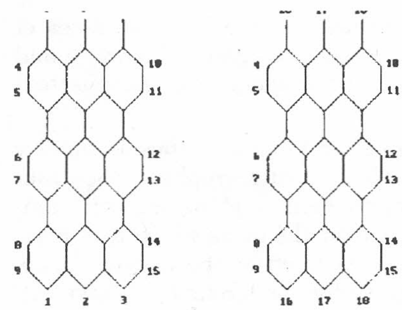
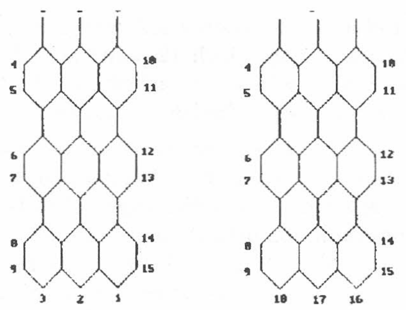


Figure 6. Creation of a torus by rolling a rectangle to a cylinder, which is then glued end to end.



Two cylinders, making a toroidal polyhex.



Two Möbius bands, making a Klein bottle polyhex.

Figure 7. Two-stage construction of genus-1 polyhexes.

Table I shows some preliminary results that compare tori with Klein bottles, where the latter seem consistently to have a higher total energy, but the same HOMO LUMO gap.

Although it does not seem especially useful, it is perhaps worth pointing out that this method *can* also be used for constructing polyhedral cages. If, as indicated, the two rectangles of Figure 8 are not formed into cylinders, but are glued immediately matching the whole perimeter of one with the other, the result is a polyhedral cage; in this case buckminsterfullerene. (See also Ref. 5).

3.4.2 *Double tori*

One or two examples of polyhex-derived double tori are given in Figures 9–11. These are 'near polyhex' structures that can be embedded on a double torus. These are probably graphs of genus 2, although this is only a conjecture which has not been proved here.

TABLE I

A comparison of some Toroidal (T) and Klein (K) bottle structures. The first seven are polyhexes and the last one an azulenoid.

Size	E_π/n		Difference	HOMO-LUMO GAP	
	T	K		T	K
16	1.457	1.537	0.080	0.828	0.828
24	1.411	1.524	0.113	0	0
32	1.441	1.544	0.103	0.469	0.469
64	1.559	1.573	0.014	0.469	0.469
84	1.572	1.575	0.003	0.494	0.494
72	1.562	1.570	0.008	0	0
80	1.558	1.573	0.015	0.351	0.351
64	1.523	1.523	*	0	0

* The difference is small and positive, appearing at the 5th decimal place of E_π/n. The eigenspectra are not the same.

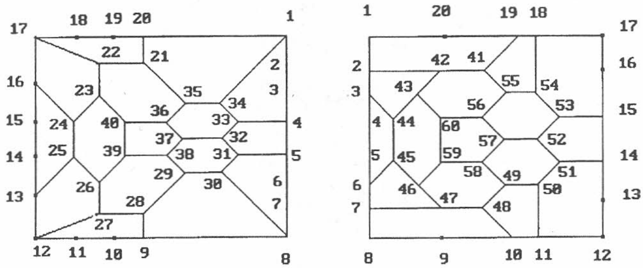


Figure 8. An unusual adjacency diagram for a polyhedron – in this case buckminsterfullerene (*cf.* Figure 7).

They are constructed by taking a toroidal polyhex, creating two holes, and gluing on a cylindrical polyhex to bridge them. There are, obviously, many possible isomers. There are at least two modes of construction, depending on whether the polyhex hole is made such as to require gluing at edges (Figures 9 and 10), or at isolated vertices (Figure 11). A number of points of interest arise. Are there other possible construction modes? For these both involve the creation of a hole larger than the perimeter of the cylinder, and involve the formation of non hexagonal 'surface' rings. More specifically, can a double torus be tessellated solely with hexagons? The method shown fails in this regard, and we have not yet thought of an alternative. From the point of view of the mathematics of a surface there is no difference in local properties when a torus is made by adding one handle to a sphere, and when one goes on to add a second handle. It is *not* clear, however, whether the same can hold true in this context of surfaces that are networks.

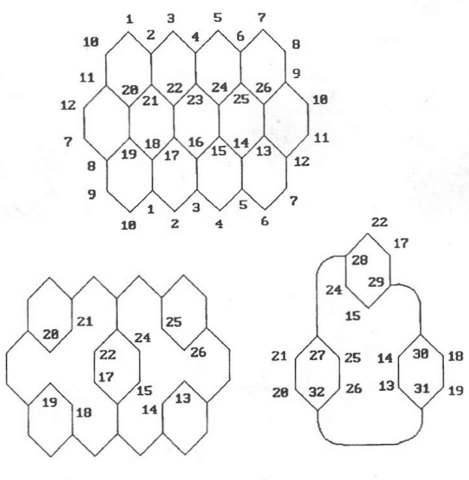


Figure 9. A simple 'near polyhex' double torus constructed by adding a polyhex cylinder to a 13-hexagon toroidal polyhex with two holes. $E\pi$ is 49.0549, compared with a range of 46.0958–50.8328 for single tori of the same size (32 vertices).

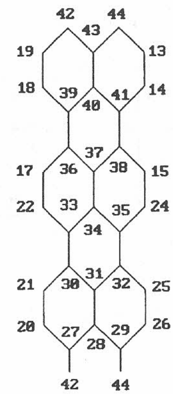


Figure 10. A larger cylinder used with the same construction method as shown in Figure 9, resulting in a 44-vertex structure, $E\pi$ 68.4490. (Single toroidal polyhex range 63.2897–70.4099)

These approaches are appealing because of the direct physical analogy, but their disadvantage (in comparison with the method used for polyhexes referred to above[3]) is that they do not so easily provide closed formulae, nor an independent means of eliminating isomorphic repeats, and sole reliance must be placed upon eigenspectra/T(G) matrices[6] for this.

The process of covering the surface of an imaginary object with a trivalent network has obvious similarities with the problem of 'tiling' as a mathematical exercise.[35–37] However, again, we have not encountered any theorems of real use for the present purpose. (For example, on the number of tilings that are possible, if stipulations about regularity or symmetry are removed). A further point is that many tiling studies are unconcerned with how many tile edges meet at a point, whereas here this is a matter of importance.

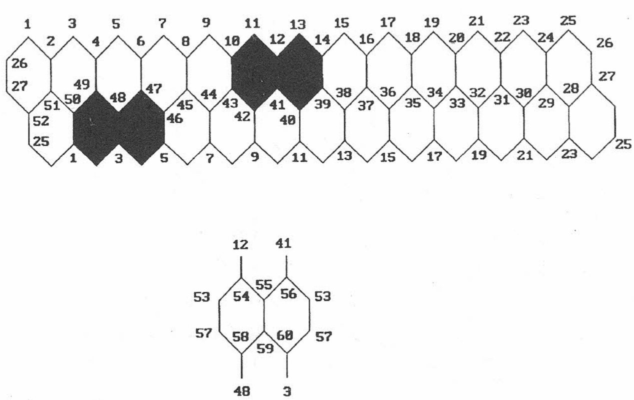


Figure 11. An alternative construction mode used to attach a cylinder to a 26-hexagon toroidal polyhex with two holes, giving a 60-vertex double torus, $E\pi$ 92.9137 (Single toroidal polyhex range 85.9175–95.9905). $E\pi$ for buckminsterfullerene is 93.1685.

4. CONCLUSION

There are many theoretically possible cage structures that may or may not eventually be seen to have a chemical realisation. There is no single technique available for recognising and classifying them. A number of approaches are in use by workers in this field, in the attempts to bring overall coherence and order to this universe of structures.

5. POST SCRIPT

Shortly after completion of this paper, recent work published from Galveston[38–40] and Ilmenau[41] became available. These studies have a different approach, but cover many of the points made here in connection with toroidal polyhexes and Klein bottles including the nature of self-intersecting surfaces.[38,40] Work is also in progress[42] on the application of molecular mechanics methods to toroidal cages.

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SAŽETAK

Primjedbe o prepoznavanju genusa i mogućih oblika kemijski zanimljivih kaveza oblika poliedra, torusa i Kleinove boce

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Dan je sažet pregled i diskusija nekih problema vezanih uz prepoznavanje i razvrstavanje struktura oblika kaveza. Razmatrane su neke nove strukture kao Kleinova boca (heskagonalna i azulenoidna) i »gotovo heksagonski« dvostruki torus.