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Cylindrical and Toroidal Polyhex Structures

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A simple graphical method is outlined for applying the encoding method developed earlier with Mallion and Pollak for polyhexes embedded in the surface of a torus. Some conditions for the occurrence of sextet 2-factorable (fully resonant sextet) and other-circuit 2-factorable structures among this series, and among cylindrical polyhex structures are pointed out. They appear more frequently here than among polyhexes on a plane, but are not such simple indicators of stability because destabilising »2n« circuits often appear too. The π-electron energy of forming small holes is calculated and compared with Hall's values for planar structures.

1. INTRODUCTION

Toroidal hydrocarbons, although as yet unknown in physical reality, have been assigned a place in at least one published classification scheme,[1] and, in the course of a comprehensive study of carbon cages,[2,3,4] a few calculations were made of resonance energies and Kekulé counts. The possibility of carbon cylinders has also aroused interest; Fowler[5] discussed a class of closed shell structures where, in effect, buckminsterfullerene has one or more bands of extra hexagons inserted around a circumference to give, for example, C_{70}, C_{84}, C_{100}, and C_{120} clusters.

A particularly intriguing feature of a toroidal polyhex is that, in contrast to networks embedded on a sphere, such as the now famous C_{60} molecule buckminsterfullerene, there need be no pentagonal rings. This predisposes one to expect a higher or at least a comparable range of stabilities. On the other hand, there are at least two factors which may run counter to this: (i) more conjugated circuits become possible in three dimensions, including ones that are destabilizing, and (ii) the geometry of a torus inevitably involves a tighter curvature around the »tube« than is the case for a sphere of the same volume. The energy cost incurred in assuming such a strained form may be prohibitive, at least for smaller structures, but this important practical point is not addressed here.

In the study of benzenoid hydrocarbons, chemists have shown particular interest in those (*e.g.* Figure 1) that can be fully drawn as an assembly of aromatic sextets connected by single bonds[6–8] (this is a special case of 2-factorability; see definitions section), and there have been several enumeration and counting studies among planar systems.[9–14] It has been remarked how few polyhexes like this there are in this class among all those theoretically possible (18 among a total of 38,742 polyhexes with ten or fewer hexagons[9]). In this paper a short preliminary exploration is made of some of the conditions for their occurrence among boundless polyhexes embedded on a cylinder or torus. The object was to gain at least some idea of how such objects compare with ordinary planar polyhexes on the one hand and with fullerenes on the other, especially with regard to the number of connectionally distinct isomers and the proportion that are, or more accurately can be, fully resonant.

The concept of circuit 2-factoring is closely related to the conjugated circuit model (see Refs. 15–17 for example) but each vertex is used only once.

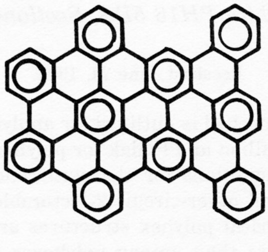

Figure 1. A sextet 2-factorable planar polyhex; inscribed circles showing fully resonant hexagons.

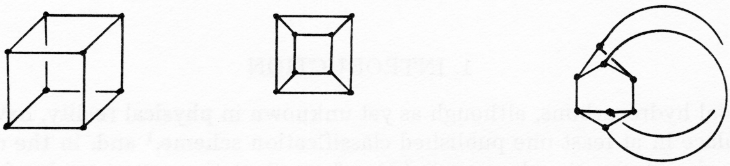

Figure 2. The cubic graph drawn as a cube; in the plane and (with obvious distortion) on a torus.

2. SOME DEFINITIONS USED

Polyhex: Here this is taken to mean any structure drawn on a surface so that it is composed of hexagons, and where any two hexagons are either disjoint or have a common edge.

Benzenoid: A 1-factorable polyhex (*i.e.* one that has Kekulé structures), and commonly the hydrogen-suppressed chemical graph of a benzenoid hydrocarbon.

There is some variability in the conventions adopted by different authors for using terms like »polyhex«, »benzenoid« and their synonyms, see for example references.[1,18,19]

Toroidal polyhex: In this paper the term is used to include any chemical graph that can be embedded in the surface of a torus as a boundless polyhex network. It is not limited by the *genus* of the graph, because it is used to include, for example, the cubic graph. This is of course planar, in the graph-theoretical sense that it can be drawn (as a pattern of rectangles) on a plane with no crossings, but it can also be drawn upon a toroidal surface as a boundless network of four hexagons (Figure 2).

1-Factor: If a graph has one, it is a set of disconnected edges drawn to include every vertex, so that each vertex has a valency of one. It is equivalent to the set of »double« bonds within a Kekulé structure.

2-Factor: If a graph has one, it is a set of disconnected rings that can be drawn to include every vertex, so that every vertex in this subgraph has a valency of two.

Sextet 2-factorable: Structures that can be 2-factored as hexagons; *i.e.* a set of disconnected hexagons can be drawn to account for every vertex. A sextet 2-factorable benzenoid is the same as a *total resonant sextet benzenoid*.[20] The former term is used here so that its scope can be extended in an obvious manner to refer to *s-circuit 2-factorable* structures.

3. CODING AND ENUMERATION

The two principle types of *cylindrical* polyhex are described in the next section, although this is not an exhaustive treatment, for at this stage we have not encoded or emunerated them systematically. A comprehensive procedure for encoding *toroidal* polyhexes and manipulating code values has been developed, which is summarized here and described in more detail elsewhere.[21]

The connectivity of a torus covered with a boundless polyhex may be characterized by a code consisting of three integers. These enable a 2 ×2 matrix to be written (one of whose numbers is always zero) defining a rectangle that repeats itself indefinitely on a planar hexagon grid and which represents a toroidal structure. The two columns of the matrix

$$\begin{vmatrix} a & b \\ 0 & d \end{vmatrix}$$

give three congruent points on the grid where the pattern starts to repeat, and defines a rectangle, as illustrated in Figure 3 for »5–2–2«. Obviously, there are various ways in which axes can be chosen, and it is necessary to decide upon a standard form. For our work we have chosen (for such a matrix, coded a–b–d) first to minimise, d, and then b. Six rules were formulated for interconversion of matrices for comparison and

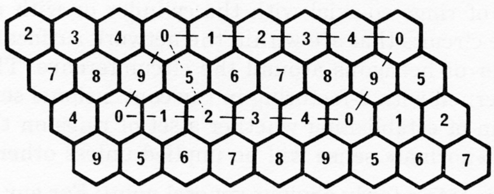

Figure 3. A 10-hexagon toroidal polyhex embedded in part of a boundless planar polyhex grid, and labelled in such a way that its code would be read as 5–2–2. The rectangle shown defines the toroidal polyhex, and is itself defined by coordinates 5,0 (from traversing 0–1–2–3–4–0) and 2,2 (from traversing 0–1–2–5–0).

reduction to a standard form.[21] In practice most toroidal polyhexes can be represented as a single strip of hexagons (a linear polyacene) with suitable connections to itself; *i.e.* usually $d = 1$ in the standard form. In this way the example 5–2–2 of Figure 3 becomes 10–5–1 on application of these rules. Alternatively, this result can be obtained simply by embedding the repeating pattern of Figure 3 on a larger network, as in Figure 4, and searching for the optimum.

The code values of toroidal polyhexes with up to 30 hexagons (60 vertices) are given in Table I. A closed formula for calculating their eigenvalues, and a simple program for constructing an adjacency matrix, was given in earlier work.[21]

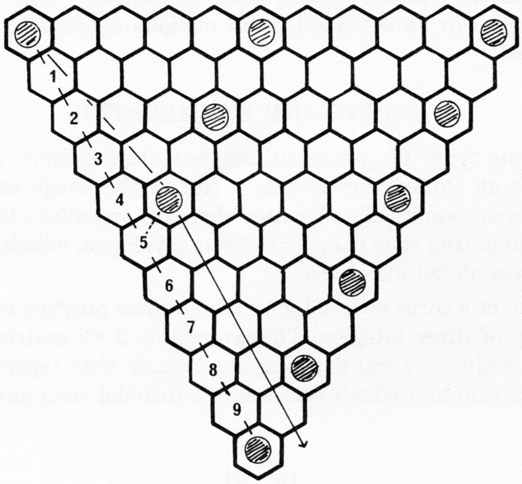

Figure 4. The same toroidal polyhex as Figure 3, embedded in a larger grid and renumbered, so that the standard code value (minimum d then minimum b in a—b—d) of 10–5–1 can be read off.

4. SEXTET AND OTHER 4n + 2 CIRCUIT 2-FACTORABILITY

The question of which structures are circuit 2-factorable is more complicated than for planar polyhexes, because the simple cylinders and tori discussed can *always* be 2-factored into a set of rings co-axial with the cylinder or with one or other axes of the torus, and (unlike circuits that are within the network surface) the size will depend simply on the number of hexagons around the circumference. The observations that follow are more concerned with 2-factoring in the conventional sense; with the usually more difficult problem of establishing whether a set of rings on the surface will cover all the vertices. This »normal« sense will be implied unless otherwise stated.

It is useful first to state a fairly obvious general point: For any polyhex, a necessary but not a sufficient condition for it to be sextet 2-factorable is that no two adjacent hexagons should contain vertices of degree two. This is because a hexagon with degree 2 vertices must be a »circled« one in a sextet 2-factor (see Figure 1), otherwise there will remain vertices that are unaccounted for, but by definition adjacent hexagons cannot both be »circled«.

TABLE I

An enumeration of toroidal polyhexes with up to 30 hexagons (60 vertices). Those that are sextet 2-factorable are starred.

6	2	1*	15	3	1	20	6	1	24	10	1	28	5	1
6	3	1	15	4	1	20	9	1	24	11	1*	28	6	1
7	2	1	15	5	1*	20	10	1	24	12	1	28	7	1
7	3	1	15	6	1	10	4	2	12	4	2*	28	8	1
8	2	1	16	2	1	21	2	1*	12	6	2	28	13	1
8	3	1	16	3	1	21	3	1	25	2	1	28	14	1
8	4	1	16	4	1	21	4	1	25	3	1	14	4	2
9	2	1*	16	7	1	21	5	1*	25	4	1	29	2	1
9	3	1	16	8	1	21	7	1	25	5	1	29	3	1
3	0	3*	8	4	2	21	8	1*	25	10	1	29	4	1
10	2	1	4	0	4	21	9	1	5	0	5	29	5	1
10	3	1	17	2	1	22	2	1	26	2	1	29	9	1
10	5	1	17	3	1	22	3	1	26	3	1	30	2	1
11	2	1	17	4	1	22	4	1	26	4	1	30	3	1*
11	3	1	18	2	1*	22	5	1	26	5	1	30	4	1
12	2	1*	18	3	1	22	6	1	26	7	1	30	5	1*
12	3	1	18	4	1	22	11	1	26	8	1	30	6	1
12	4	1	18	5	1*	23	2	1	26	13	1	30	7	1
12	5	1*	18	6	1	23	3	1	27	2	1*	30	8	1*
12	6	1	18	9	1	23	4	1	27	3	1	30	9	1
6	4	2*	6	0	3*	23	5	1	27	4	1	30	10	1
13	2	1	19	2	1	24	2	1*	27	5	1*	30	11	1*
13	3	1	19	3	1	24	3	1	27	6	1	30	12	1
13	4	1	19	4	1	24	4	1	27	9	1	30	15	1
14	2	1	19	8	1	24	5	1*	9	3	3*	15	5	2
14	3	1	20	2	1	24	6	1	9	6	3*			
14	4	1	20	3	1	24	7	1	28	2	1			
14	7	1	20	4	1	24	8	1*	28	3	1			
15	2	1*	20	5	1	24	9	1	28	4	1			

4.1. Cylindrical Polyhexes

We consider here two principal classes of cylindrical polyhex, distinguished by the orientation of hexagons with respect to the axis of the cylinder, see Figure 5. (These are not the same as the carbon cylinders already referred to that were discussed by Fowler.[5]) Both kinds are related to polyhex near-rectangles, and a traverse of any cylinder end must visit a repeating sequence of either degree-2···degree-3··· or degree-2···degree-2···degree-3···degree-3 vertices.

4.1.1. Cylinders of type 5a *cannot* be sextet 2-factored in the ordinary sense because adjacent hexagons on the end perimeters contain vertices of degree 2. However, note that (i) if promontories are formed by adding hexagons to the ends at suitable positions (*e.g.* Figure 1, if is »wrapped around« with suitably added edges) then the whole may be sextet 2-factorable, and (ii) as mentioned above, a cylinder of type 5a can be 2-factored into a set of rings threaded onto the cylinder (Figure 6). For these to be of $4n + 2$ type, there must be an odd number of hexagons around the circumference.

4.1.2. Cylinders of type 5b may be sextet 2-factorable, depending on their dimensions, and provided that the number of polyacene strips parallel to the axis is even (see 4.1.3. below). The smallest such structure has four hexagons (Figure 7). This kind of cylinder must have polyacene strips parallel to the axis that are all of the same size, a

b

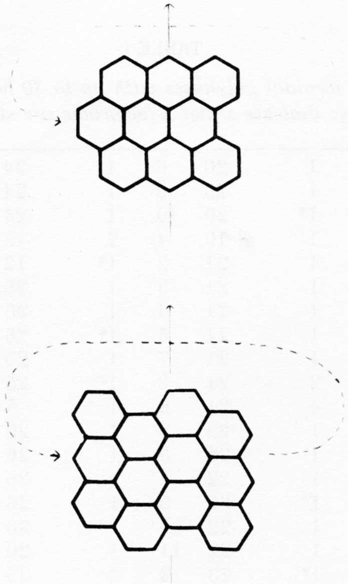

Figure 5. Two types of cylindrical polyhex considered.

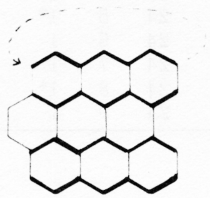

Figure 6. A special kind of circuit 2-factoring (heavy lines) shown by cylindrical polyhexes of type 5a.

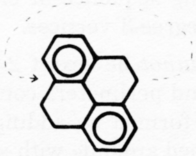

Figure 7. The smallest truly cylindrical sextet 2-factorable polyhex.

or that are interleaved with strips differing in length by one hexagon. When circuits co-axial with the cylinder are considered, it can be seen that each double hexagon strip unit contributes four vertices to such a circuit, so that they are all of the $4n$ type. It therefore follows that geometric strain, and the attenuation of destabilising coaxial circuit effects by increased size, both indicate that a comparatively large diameter would be needed for any stable structure of this kind to exist.

4.1.3. A cylindrical polyhex of type 5b with an odd number of polyacene strips parallel to the axis cannot be sextet 2-factored in the ordinary sense. This is because if there is an odd number of polyacene strips, then on each cylinder end there must be at least one pair of adjacent hexagons which both have degree 2 vertices.

This restriction does not apply to larger circuit factoring; for example, Figure 8 shows a 10-circuit 2-factoring in a cylinder with three rows of four hexagons.

4.1.4. For a cylindrical polyhex of type 5b with an even number of polyacene strips parallel to the axis, let k be the number of pairs of strips, h the total number of hexagons, and s the size of $4n + 2$-circuit $(6,10,14,18,\cdots)$ being considered. Each pair of polyacene strips may have two rows that are equal in length or that differ by one hexagon. Then the structure will be s-circuit factorable if

$$h = k(s/2 \times i - 2)$$

where i is a positive integer.

Setting $s = 6$ and $i = 1$ gives the degenerate case of (sextet 2-factorable) circúlar poly para-phenylenes (Figure 9). Figure 10 illustrates the first few members of this series. It can be seen that such a cylinder is both 6- and 10-circuit factorable when there are 13 hexagons (greatest depth 7), and 6-, 10- and 14-circuit factorable when this at 105 hexagons (the lowest common multiple of 3,5,7).

4.1.4. A cylindrical polyhex of type 5b with an even number of polyacene strips parallel to the axis is s-circuit factorable on the surface if and only if the number of vertices in divisible by s. That this is a necessary condition is obvious by definition.

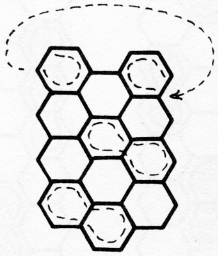

Figure 8. A cylindrical polyhex of type 5b but with an odd number of linear polyacene strips parallel to the axis. These are not sextet 2-factorable, but this example is 10-circuit 2-factorable.

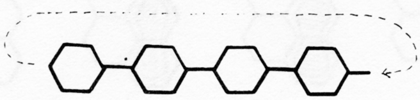

Figure 9. One of the degenerate class of shallowest possible sextet 2-factorable »cylindrical« »polyhexes«.

That it is sufficient may be seen by referring to Figure 10. Each hexagon added to a cylindrical polyhex of n vertices is responsible for increasing the number of vertices by two. The only way of adding $s/2$ hexagons (giving $n + s$ vertices, also a multiple of s) whilst remaining a cylinder of type 5b results in an s-circuit factorable structure.

4.1.5. The examples of s-circuit 2-factoring shown here all relate to the perimeter of *linear* polyacenes. Perimeters of non-linear catacondensed polyhexes (for example phenanthrene) can also appear as 2-factors, but we do not know how many and which others are available.

4.2. Toroidal Polyhexes

4.2.1. A toroidal polyhex of code a–b–d (see section 3) is sextet 2-factorable if and only if 1) a MOD 3 = 0 and 2) $(b + d)$ MOD 3 = 0. This is seen by considering a sextet 2-factored infinite hexagon lattice. (*E.g.* Figure 1 where the internal pattern continues indefinitely.) Any given hexagon is either circled or not circled. Starting with an empty uncircled lattice, if any hexagon is circled, then the condition of every other hexagon

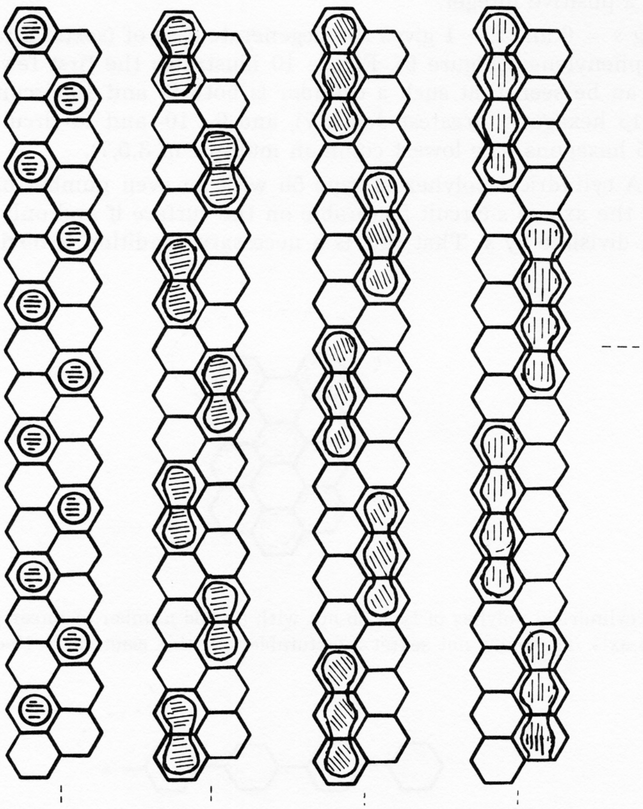

Figure 10. The unit vertical strip of a cylindrical polyhex of type 5b, shown with four different circuit 2-factorings. The cylinders can be extended to infinite depth and to infinite circumference.

is fixed (but note that this does not apply if it is specified as uncircled). For any hexagon there are three ways of drawing a line passing through the centre, perpendicular to two edges. On a sextet 2-factored structure such as Figure 1, any such line traverses a repeating sequence of one circled and two uncircled hexagons. Furthermore, this is still true if the line changes direction, so long as it does so by 120°. It follows that the number of hexagons traversed in going from any circled and labelled hexagon to another with the same label is a simple multiple of 3. In the code *a–b–d*, a is the number of hexagons in each row (*i.e.* position of the first repeated hexagon on straight line), and $b + d$ represents the number of hexagons traversed to find the same labelled hexagon on the other axis.

4.2.2. As a matter of general interest we note that these toroidal polyhexes all have Kekulé structures (1-factors). This can be proved by considering deletion of one of the three sets of parallel edges; the resultant subgraph is a 2-factor. Since the toroidal polyhex is cubic and is, therefore, its own branching graph,[22] and since there is a one–to–one correspondence between the 2-factors of a graph and the 1-factors of its branching graph[22,23] the toroidal polyhex is 1-factorable and has Kekulé structures.

4.2.3. Table I shows all the toroidal polyhexes with up to 30 hexagons (60 vertices), and shows which are sextet 2-factorable. These amount to 27 (19%) out of a total of 141 with 30 or fewer hexagons. This is a higher proportion than for planar polyhexes as a whole,[9] though more comparable with the behaviour of »constant isomer series«.[20]

5. DESTABILIZING CIRCUITS

Care must be taken in attempting to assess the relative effects of stabilizing ($4n + 2$) and destabilizing ($4n$) circuits, since the former are usually essentially coplanar, while the latter are definitely not, but qualitatively at least, their effects will tend to oppose. The presence of $4n$ circuits differentiates the three dimensional structures from planar polyhexes, where only $4n + 2$ circuits occur. By analogy with the theory of Clar resonant sextets, it is probably the case that destabilisation is greatest when a structure can be 2-factored into a set of independent $4n$ rings, and this is often coincident with a more »benign« 2-factorability. The 6-vertex graph shown in Figure 11, for example, is 2-factorable into either two hexagons or three four membered rings.

The prevalence of this effect has not been investigated systematically, but it (and indeed the presence of either kinds of circuit) can conveniently be studied graphically. Using the repeating planar representation described (*e.g.* of toroidal polyhex 10–5–1

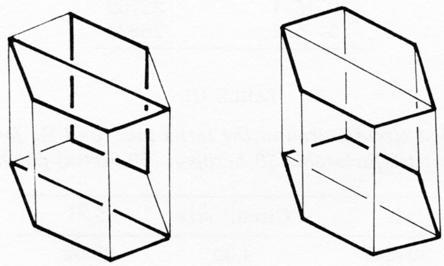

Figure 11. A 12-vertex graph that can be 2-factored as either two hexagons or three 4-circuits.

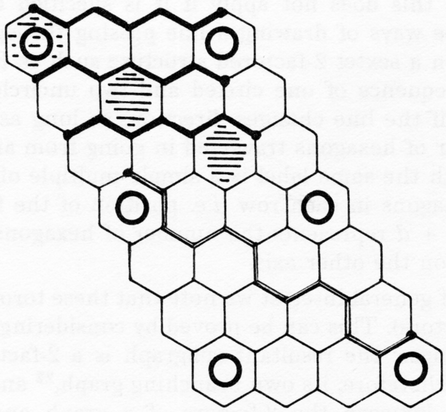

Figure 12. Toroidal polyhex 3–0–3, showing selected circuits. Circles show the hexagon arbitrarily chosen as the origin, and their pattern repeats indefinitely on this planar representation of the toroidal surface. The hatched hexagons form a possible sextet 2-factoring on the toroidal surface, while heavy lines indicate a possible circumferential sextet 2-factoring. The double lined path shows one circumferential 12-circuit. (There cannot be a 12-circuit 2-factoring because the number of vertices, 18, is not a simple multiple of 12.

TABLE II.

The square root of the tail coefficient of the characteristic polynomial for the 30 hexagon, 60 vertex, toroidal polyhexes.

Code	$\sqrt{a_n}$
30– 2–1	0
30– 3–1	95139
30– 4–1	25344
30– 5–1	0
30– 6–1	21483
30– 7–1	21483
30– 8–1	0
30– 9–1	17019
30–10–1	3069
30–11–1	0
30–12–1	16128
30–15–1	32769
15– 5–2	26829

TABLE III.

Smallest circuits around the torus tube, and E_π for the four sextet 2-factorable 30 hexagon (60 vertex) polyhexes.

Code	Circuit size	$E_\pi{}^{21}$
30–2–1	4,30	85.92
30–5–1	10,12	93.52
30–8–1	8,16	92.93
30–11–1	6,20	93.06

in Figure 4), a »normal« circuit, within the surface and which must be of $4n + 2$ type, is represented by an obvious graph circuit drawn to join up adjacent vertices. An »abnormal« circuit, on the other hand – which girdles the three dimensional tube of the torus, and which may be of $4n + 2$ or $4n$ type – has to be drawn as a path from some labelled vertex to where the same vertex appears again (see Figure 12).

Different circuits contribute to the algebraic structure count,[18] and the effects of this in rendering the tail of the characteristic polynomial unreliable as a simple indicator of the Kekulé count (and therefore of resonance energy) is shown for the 30 hexagon C_{60} series in Table II. The smallest circumferential circuits of members of this series that are sextet 2-factorable are shown in Table III, and are consistent with the view that $4n + 2$ or $4n$ circuits stabilize or destabilize, respectively, in inverse proportion to their size (this ignores their *practical* effectiveness arising from the amount of orbital overlap).

On the other hand, although 30–5–1 appears from this to be the most favoured sextet 2-factorable structure, the highest E_{π} value for the series is for 30–3–1 (95.99). This, although it does not have a full set of resonant sextets, is 10-circuit factorable in the conventional sense, and has a set of circumferential 6-circuits.

6. HÜCKEL π-ENERGY OF CYLINDRICAL AND TOROIDAL FORMS

An alternative approach to seeking some illumination of the possible stabilities of these structures is to ask – what is the effect upon the π-energy of a planar polyhex of »wrapping it around« to form first a cylinder and then a torus? This intuitively intriguing question is not easy to answer satisfactorily, because it is difficult to compare like with like. One cannot form a polyhex torus by simply adding edges to connect the opposite sides of a planar polyhex without introducing non-hexagonal-rings on the surface, for any planar representation of the polyhex »skin« of a toroidal polyhex will differ in the number of its vertices or of its rings. Even a cylinder cannot be formed in this way if it is to conform to type 5a or 5b. The difficulty is illustrated by Figure 13. As a practical aid to visualisation it is perhaps useful to point out that a convenient mental construction process, corresponding to the planar tessellations used (Figure 14) is *coalescence*, where pairs of same-label vertices and edges are »folded over« and fused.

We have briefly investigated an example by two complementary approaches in order to give some idea of the magnitude of the effects involved, and the results are

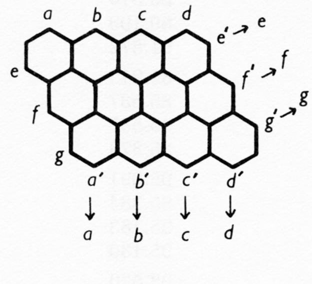

Figure 13. A cylinder can be made by making the connections $a - a'$, $b - b'$, $c - c'$, and $d - d'$, or $e - e'$, $f - f'$ and $g - g'$, but in either case the bridging row of hexagons will be a short row. If both sets of connections are made (forming a torus), the »corner« rings will be non-hexagonal.

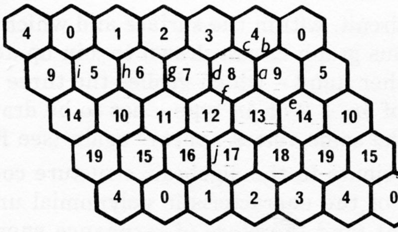

Figure 14. Toroidal polyhex 20–5–1 with one unit shown lightly shaded (actually written here as 5–0–4; see Section 3).

TABLE IV.

The effect on the total π—energy of a 38-vertex, 12-hexagon polyhex rectangle (Figure 13), of conversion, first to a cylinder and then to a (non-polyhex) torus.

	E_π	Change in E_π per extra edge
A(3x4) 12 hexagon planar rectangle (Figure 13).	54.973	
Cylinder by *e–e′, f–f′, g–g′* linking.	56.725	0.584
Cylinder by *a-a′, b-b′, c-c′, d-d′* linking.	56.986	0.503
A torus formed by both the above linkings.	59.191	0.603
A cylinder made by side linking of 12-linear polyacene.	70.794	0.067
A »cylinder« made from 12 hexagon poly para-phenylene	100.278	0.396

TABLE V.

*The effect on the total π-energy of some toroidal polyhexes of deleting certain edges. *See Section 3 for an explanation of the code.*

Structure*	Deleted edges	E_π	E_π difference per deleted edge
20–5–1	None	63.098	
	a	62.307	0.791
	b	62.497	0.628
	c	62.370	0.727
	a,d	61.4573	0.820
	b,e	61.8241	0.637
	c,f	61.627	0.736
	a,d,g	61.608	0.830
	a,d,g,h	59.810	0.822
	a,d,g,h,i	59.199	0.780
	a,j	61.572	0.736
30–2–1	none	85.919	
	one	85.537	0.382
	one	85.537	0.382
	one	85.878	0.041
30–3–2	none	95.991	
	one	95.384	0.606
	one	95.183	0.807
	one	95.130	0.861
30–5–1	none	93.520	
	one	93.017	0.503
	one	93.026	0.493
	one	93.024	0.496

shown in Tables IV and V. In the first we take a twelve-hexagon, 38-vertex polyhex rectangle and convert it to a cylinder by adding edges, thus forming extra hexagons, but no extra vertices. The wrapping can be done in either or both of two senses. If both are done together the resulting object is a toroidal structure but, as mentioned above, it is not a toroidal *polyhex*, since the rings embedded in the surface are not all hexagons. For comparison, the effects of linking up the two ends of a poly para-phenylene, or the two longer sides of a twelve hexagon linear polyacene, are shown, although the latter is likely to be atypical because four membered rings are formed.

As a complementary approach, Table I shows the effect on E_π of deleting certain edges from a already formed toroidal polyhex. The values vary from structure to structure, and within a given structure there are three kinds of edge incident at any vertex, depending on orientation. Within this limited sample there is much more variability than was found by Hall[24] in an interesting study of two planar polyhexes (with ten and seventeen hexagons). He found that deleting an edge resulted in a fairly constant energy difference of 0.64 beta units. The variability presumably arises from differences in the circuits being disrupted. In Table III, the structures that are associated with the smallest average energy difference (30–2–1 and 30–5–1) are those that are sextet 2-factorable.

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SAŽETAK

Heksagonske strukture na cilindru i torusu

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Izložen je jednostavan grafički postupak za primjenu koda, razvijenoga ranije u suradnji s Mallionom i Pollakom, na heksagonske strukture, smještene na površini torusa. Istaknuti su neki uvjeti koje ove strukture, kao i heksagonske strukture smještene na cilindru, moraju zadovoljiti da bi posjedovale 2-faktor od samih šesteročlanih ili općenito n-teročlanih prstenova. Iako se ovo svojstvo češće sreće kod struktura smještenih na torus ili cilindar nego kod onih smještenih na površinu, ipak je diskusija o stabilnosti otežana zbog istovremene pojave velikog broja destabilizirajućih $4n$-teročlanih prstenova. Izračunane su (π-elektronske) energije potrebne za stvaranje šupljina u heksagonskim strukturama smještenima na torusu i cilindru te su uspoređene s Hallovim vrijednostima za strukture smještene u ravnini.