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Charting the ocean of fully resonant azulenoids: a few navigational pointers

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ABSTRACT

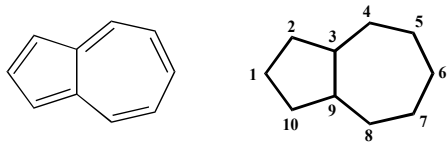
Some properties of fully resonant azulenoids are compared with those of related benzenoid and other arenoid structures. They are not particularly easy to deal with in terms of convenient, transparent and concise structural encoding, although, since they all have a multiple of ten vertices, by always numbering vertices in the same way around each azulene, an unusually informative connection table may be generated. On the other hand, certain sub-classes can be concisely encoded, most notably certain toroidal forms that have a constant inter-azulene connection pattern, by matching them to appropriate fully resonant toroidal benzenoids used as templates.

1. INTRODUCTION

1.1 Definition

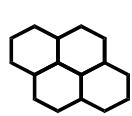
The azulene graph is a pentagon-heptagon pair, with one edge in common, that can represent the bicyclic $C_{10}H_8$ hydrocarbon azulene (Figure 1). Examples of a fully resonant benzenoid and a fully resonant azulenoid are shown in Figure 2. The defining characteristic of the azulenoid is that a set of azulene subgraphs (referred to hereafter as 'azulenes') can be traced in disjoint fashion to account for all the vertices. In chemical terms the essential notion

used is a system that can, but need not, be drawn as a set of fully conjugated azulene nuclei interconnected by single bonds.

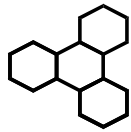


(a) (b)

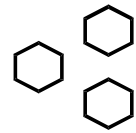
Figure 1. *Azulene in its usual representations as a conjugated hydrocarbon* (a)*, and as a chemical graph* (b). (*The vertex labelling used here differs from normal chemical convention.)*

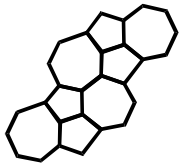


A benzenoid.

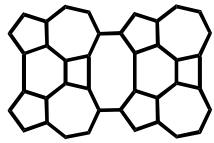


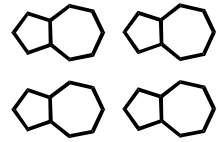
A fully resonant benzenoid, where every vertex is part of a disjoint benzene (hexagon).





An azulenoid.





A fully resonant azulenoid, where every vertex is part of a disjoint azulene (pentagon-heptagon pair).

Figure 2. *Example of a fully resonant benzenoid and a fully resonant azulenoid.*

1.2 Some points of comparison with benzenoids

The networks discussed here can be considered analogous to the well known fully benzenoid or fully Clar structures (Figure 2). Many have worked in this area[1-11] and on the generalised concept of fully arenoid structures.[3, 12-18] The references cited here are examples, but

represent only a selection of relevant papers. In the case of both benzenoid and azulenoid species of this class, two sets of rings or faces may be distinguished: those that constitute the defining set of disjoint rings, said to be the *full* set, and those that do not, the *empty* set. There are, however, some differences to be noted.

(i) Every ring of a fully resonant benzenoid, whether full or empty, is a hexagon, but it can easily be verified that fully resonant azulenoids that are extensible in two dimensions cannot be constructed from pentagon-heptagon pairs alone, and so the azulenoid networks directly analogous to a polyhex or graphitic sheet, namely pentaheptites,[19] cannot be fully resonant in an azulenoid sense.

(ii) While both benzenoids and azulenoids that are fully resonant have 2-factors consisting of a single cycle size (six and ten respectively), the corresponding 2-factor is sufficient to define the benzenoid but not the azulenoid case, because of azulene's bridging edge (3-9 in Figure 1.) In fact the fully resonant azulenoids are rather more akin to fully resonant naphthalenoid structures.[14, 17]

(iii) However, while some fully naphthalenoids are essentially disconnected, and therefore fall into the narrow class suggested by Knop et al.,[20] these fully resonant azulenoids do not, for the fully conjugated azulene nuclei can be, but are not required to be, connected to others by single bonds. This is illustrated with an example in Figure 3. We thus follow the (perhaps more widely used) general application of the concept, in which essential disconnection is a special case. In fact we formulate the following conjecture.

Conjecture 1: No fully resonant azulenoid as defined in this paper is essentially disconnected.

(iv) Planar fully resonant azulenoids have a number of elementary mathematical properties that are very similar to those recorded for planar benzenoids in general,[21] but some small differences are noted here. In this context, the number of vertices of degree three is not affected by a change of ring size alone, but clearly the number of degree-two vertices *is* so affected. A correction parameter ($\Delta = \sum (\text{Ring size} - 6)$) is therefore applied to take account

of deviations from six of ring sizes. The resultant equations, and their application to two azulenoid examples, are shown in Table 1.

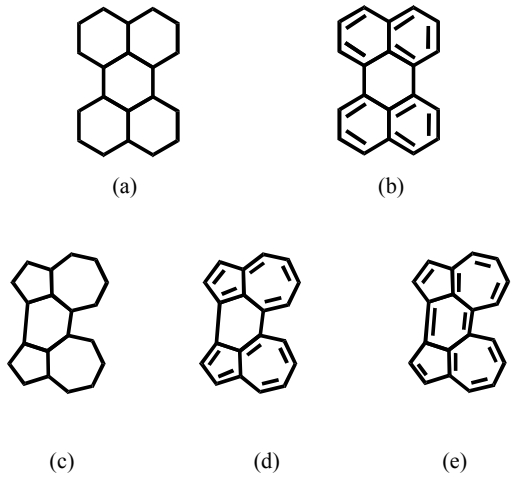


Figure 3. *An example of where an azulenoid differs from its similarly-structured naphthalenoid counterpart. The fully naphthalenoid (a) has nine 1-factors (Kekulé structures) including (b), but in no case is either of the inter-naphthalene bridging edges involved, so that the two naphthalene units are said to be essentially disconnected.*[27] *The fully resonant azulenoid (c), however, besides structures of type (d) can also be drawn as (e), and therefore is not essentially disconnected. See Conjecture 1.*

When computing the value of Δ, the fully resonant azulenes can be ignored, since each unit is equivalent to two hexagons. It follows that when the empty rings are all hexagons, (e.g. Figure 4), this is a special case and requires no adjustment. It can be treated as a benzenoid – as if every ring were a hexagon.

1.2 Nomenclature

Clar and Zander[1] introduced the concept of fully benzenoid structures, and since then many papers have been written on this and the extended concept of fully arenoid structures, using various terminologies. Here we point out that work reported here originally started[16] with use of the term 'fully azulenoid', in obvious parallel with 'fully benzenoid'. Subsequently

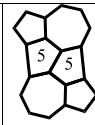
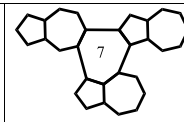
						
Parameter	**Equation for benzenoids[21]**	**Equation for non-benzenoids**	**Values**	**Σ**	**Values**	**Σ**
Δ (correction parameter)		$\sum$ (Ring size – 6)	-2		1	
# vertices, *n*	$4h+2-n_i$	$4R+2-n_i+\Delta$	24+2-4-2	20	28+2-1+1	30
# edges *m*	$5h+1-n_i$	$5R+1-n_i+\Delta$	30+1-4-2	25	35+1-1+1	36
# edges *m*	$n+h-1$	$n+R-1$	20+6-1	25	30+7-1	36
# v_3 internal	n_i	n_i	4	4	1	1
# v_3 external	$2h-2-n_i$	$2R-2-n_i$	12-2-4	6	14-2-1	11
# v_3 (total)	$2h-2$	$2R-2$	12-2	10	14-2	12
# v_2 (external)	$2h+4-n_i$	$2R+4-n_i+\Delta$	12+4-4-2	10	14+4-1+1	18
# edges, internal	$h-1+n_i$	$R-1+n_i$	6-1+4	9	7-1+1	7
#(3,3)-edges, external	b	b		2		4
# (2,2) edges	$b+6$	$b+6+\Delta$	2+6-2	6	4+6+1	11
# (2,3)-edges	$4R-4-2b-2n_i$	$4R-4-2b-2n_i$	24-4-4-8	8	28-4-8-2	14
Perimeter size = *v* external = *m* external	$4h+2-2n_i$	$4R+2-2n_i+\Delta$	24+2-8-2	16	28+2-2+1	29

Table 1. *Comparison of some simple relationship formulae for benzenoids[21] and non-benzenoids, with two worked examples for the latter. Each system has n vertices (n_i of them internal) and m edges. Benzenoids have h hexagons, while non-benzenoids have R rings of variable size.*

however, it seemed better, if somewhat clumsy, to expand the term to 'fully resonant azulenoid', to avoid confusion with structures that are merely tilings by (non-disjoint) azulenes,[18, 19] often called pentaheptites, but which have sometimes been referred to as being fully azulenoid.[19] In this context there is a precedent for the term 'resonant' in the work of Dias, who has referred to, for example, 'total resonant sextet benzenoid

hydrocarbons'.[9] Dias also used the term 'azulenoid', (as we did later, for pentaheptite structures or fragments).[22] In what follows, by default the term 'network', when unqualified, means such a fully-resonant-azulenoid network.

1.3 Generation

Extensive work on programs for generating 3-valent networks in general has been done by others; by Brinkmann and Dress[23] for example. For this particular subset, besides systematic enumeration of the connection possibilities for very small systems, or simply drawing by trial and error, the author has found two specific methods to be fruitful. These are (i) rotation of subgraphs within certain larger subgraphs of a benzenoid network (in the manner of the Stone-Wales transformation) and (ii) conversion of an existing fully resonant networks by 'sliding' rows of azulenes relative to one another.[16, 18] Although this involves an element of subjective judgement, we know of no currently available method that both is simple to visualise, and exhaustive of all possibilities.

1.4 The motivation for this study

Among benzenoids, the possibility of drawing them as fully resonant structures is associated with a tendency to be more stable. Since azulene is often regarded as being at least to some extent aromatic,[24, 25] like benzene, this provides one motive for investigating the properties of such networks. A second one stems from the fact that azulene itself has a modest dipole moment and some tendency – no more than that – to polarise by electron drift from the seven to the five membered ring, especially under reacting conditions. This fact is often rationalised in simple Hückel terms as an attempt by azulene to reorganise itself into a pair of (oppositely charged) aromatic sextets analogous to naphthalene. It has the obvious, although at present only speculative, implication that there might be interesting features of both the chemical and electrical properties of such networks, and of any tubes or fullerene-like objects related to them.

Such questions are not addressed here, where the objective is merely to explore some elementary connectional and computational properties of this group, and since fully resonant azulenoids in general do constitute a well-defined subgroup within the very many conceivable polycyclic networks and structures, there seems in any case to be some value in attempting to extend their characterization.

2 DISCUSSION

2.1 Some properties of fully resonant azulenoid networks

2.1.1 The local environment of an azulene within a fully resonant structure.

As already implied, these networks are more complicated to characterise than the corresponding benzenoid structures, partly because the lower symmetry of azulene (in comparison with benzene) results in less degeneracy among possible isomers. Its periphery is not uniform like a hexagon, and the internal bridging edge of azulene means that vertices capable of accepting a connection from another azulene are not all equally spaced around the 10-membered ring. Furthermore, in contrast to benzenoids, even planar drawings suffer geometrical distortion of some regular polygons.

The internal area, i.e. the region that is unaffected by the details of any periphery present, has only one possible ring pattern in the case of a fully resonant benzenoid. These networks, on the other hand, can have several. For example, at least eight ways of forming a uniform network containing parallel rows of azulenes that are 'head to tail' are known.[18]

Intuitively, the simplest kind of azulenoid network of this class is where the disjoint azulenes are all within what otherwise is a polyhex sheet, and it is apparent that this can be drawn in only one way, that has parallel rows of head-to-tail azulenes in alternating orientations (Figure 4 and Theorem 1). Here too, in geometric representations, the hexagons can be regular only at the expense of distorting the five and seven membered rings, or vice-versa.

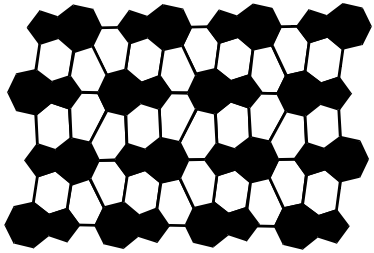


Figure 4. *The ring pattern of what is, arguably, the simplest type of fully resonant azulenoid. The empty rings are all hexagons*.

For the purpose of drawing intermediates and building up such structures in general, it is useful at this point to make explicit, four obvious consequences of the definition given for a fully resonant azulenoid in Section 1 above:

(i) Every connection radiating *from* one azulene can go only *to* another azulene.

(ii) Any vertex that is connected to more than one azulene is forbidden – because it can then be incorporated into another azulene only by making two azulenes contiguous.

(iii) Within the interior of these networks, unless they are to be highly strained and 'artificial', each azulene is connected to at least three, preferably at least four, and at most eight other azulenes. (By disregarding apparent geometric plausibility altogether, some, but not all, could be connected to only two others.) The upper bound of eight represents the number of vertices that are of degree two, and therefore available for connection, within each azulene.

(iv) The size of an empty ring is at least four, and is formed when an edge between two vertices of degree two from each of a pair of azulenes is adjacent, and therefore connected, to the other. It cannot be three whilst keeping the degree of all vertices to no more than three. The upper limit of ring size is indefinite and depends upon the size and shape of the system as a whole because, just as a structure that locally is of the benzenoid type may have 'holes' – i.e. rings larger than a hexagon (a class generally known as the coronoids[26]) – so these networks also may have large inner rings. See Figure 5 as an example.

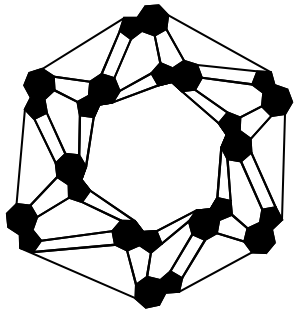


Figure 5. *A planar fully resonant azulenoid centred on an 18-gon. It is analogous to a coronoid*.

Theorem 1: There is one and only one fully resonant azulenoid pattern where every empty ring is a hexagon (see Figure 4).

A proof of this may be established pictorially: see Figures 6 and 7. There are only two ways in which two azulenes and one hexagon may be drawn as fully resonant azulenoid; namely by connecting equivalent positions either side of the internal azulene bridge so that the azulene directions either match or oppose. (See Figures 6(a) and 7(a), where such a pair of azulenes is also surrounded by hexagons).

Consider the matching case first (Figure 6). Here the pair of azulenes can be extended upwards or downwards in the same way, but all attempts to extend the structure to the right or the left result in either forbidden vertex or non-hexagonal ring formation, exemplified by 6(b,d, and e).

In the opposing case (Figure 7), the initial pair may again be extended upwards or downwards. Extension to right or left works, but only by matching each new azulene to the direction of its horizontal neighbour.

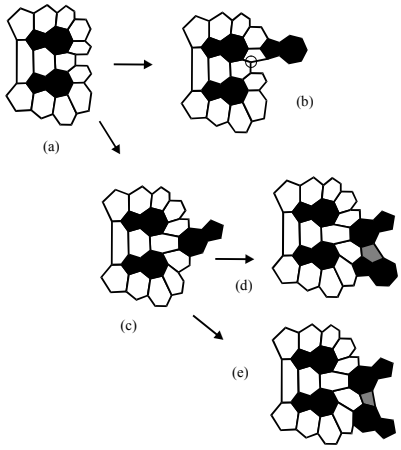


Figure 6. *A stacked pair of azulenes of the same orientation can be surrounded by hexagons, and can be extended indefinitely up or down, but horizontal extension does not work, for it results in forbidden vertices (circled) or non hexagonal rings (shaded).*

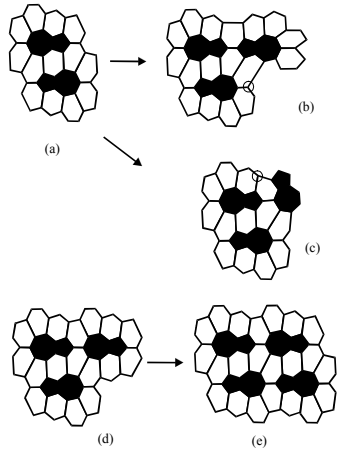


Figure7. *An opposing pair of azulenes can be extended in every direction, provided the azulenes in each row all have the same orientation.*

2.1.2 The global environment of an azulene within a fully resonant structure

Because these networks vary in their ring composition (2.1.1) they can be tailored to cover a wider variety of surfaces than is the case for benzenoids. As is well known, benzenoids, whether fully resonant or not, can be embedded in, among others, the plane, and the surfaces of a cylinder, torus or Klein bottle, but not the sphere. A fully resonant azulenoid can be embedded on all these *and* on a sphere, although not with an all-hexagon empty ring set: For example, Figure 8, if duplicated and suitably glued, gives this result.. These, roughly hemispheroidal, structures were earlier suggested[27] as possible tube cappings. If the radius of the disk shown in Figure 8 is extended by adding concentric rings of azulenes in the same manner, the structure remains topologically planar, but in the plane it is highly distorted,[18] and its apparent natural geometry is that of a half capped tube, with rows of azulenes along its length, separated by a 4-6-8 pattern of empty rings. This example also shows a case where an azulene has maximum connectivity, in being connected to eight other azulenes. Tubular junctions too have been shown to be coverable with such fully resonant networks.[28]

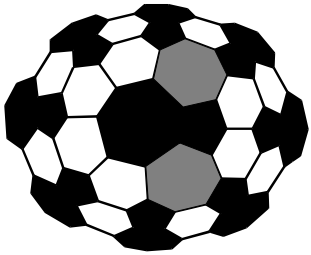


Figure 8. *Perspective view of a fully resonant azulenoid cap or hemisphere. Note that the central azulene has two heptagons among the set of eight empty rings that surround it*.

3. ENCODING, RECOGNITION AND RETRIEVAL

The structural information being discussed here is connectivity, given in full by the adjacency matrix or, more concisely, by a connection table. This is, however, relatively bulky to store, and recovery of the structure from this information, while quite straightforward, is, in general, not particularly easy.

3.1 Benzenoids versus fully resonant azulenoids

At least two groups of benzenoids are straightforward to encode: conventional planar benzenoids can be fully characterised by the boundary code[29] (a simple string of digits, each within the range 1 – 6), while toroidal benzenoids require merely a string of three integers that defines a notional quadrilateral assembly of hexagons that can be rolled up and glued to form the torus in question.[30, 31] Mention should also be made of the beautiful scheme for classifying benzenoids – a periodic table – introduced by Dias,[32-34] and extended to other polycyclic systems.[22] Such schemes encompass, of course, total resonant sextets.[8, 9]

However, matters are still not entirely straightforward with the networks described here, for the reasons outlined earlier. There is, though, one obvious characteristic of this class that may be used to considerable advantage, namely, that the azulene graph has ten vertices – and ten is the base usually used for human arithmetic. This means that by a careful choice of labelling, the connection table (representing the adjacency matrix) can be rendered considerably more intelligible and informative than is usually the case.

3.2 Procedure for constructing an abbreviated connection table for any fully resonant azulenoid

1. First give numeric labels to all *azulenes* in sequence, starting from zero. The order is immaterial, although it may be helpful to adopt some consistent procedure whereby near neighbours have consecutive numbers as far as possible.

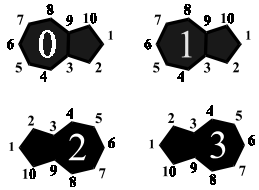
2. Taking azulenes in the same sequence, number the *vertices* of each one consecutively around its periphery in a standard manner, say clockwise from a certain position (see Figure 1.), but this time starting from one. Thus the first vertex of azulene-zero is labelled 1; the first vertex of azulene-one is 11; that of azulene-two is 21, and so on.

3. Define the inter-azulene connections.

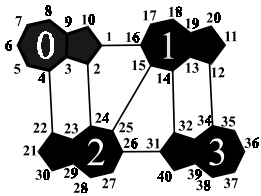
The procedure is illustrated in Figure 9. The details of step (a) are arbitrary, and show the convention we have adopted, but they must in any case be standardised. In practice, one will not implement step (a) explicitly; it is shown here only for clarity. Having adopted this procedure, it is relatively easy to recover structural information from a connection table that is written from such a diagram, because, given a vertex labelled *v* we know immediately that

the azulene it belongs to is labelled as the integer division result $\{(v\text{-}1)/10\}^*$, and that the relative local position of this vertex on this azulene (now identified by the label a) is (v-10a): both are trivial calculations and readily apparent to the eye.

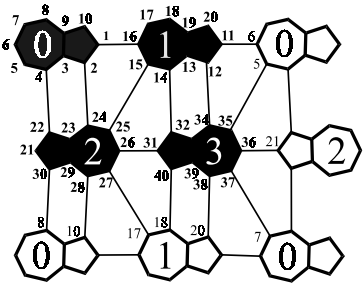
Note that we always start numbering from the same local position on the azulene. By specifying the direction (clockwise), every position is then unambiguous, but the position 1 chosen here (it could have been 6) is *more obviously* unambiguous as a starting point.



(a) Label the azulenes from zero, and the vertices within each one from 1, going clockwise from the same position.



(b) Mark inter-azulene connections and convert the vertex numbering to a global sequence.



(c) Since this is a torus, draw enough of the biperiodic pattern to enable completion of all the edges of the torus.

Figure 9. *Constructing the connection diagram for a fully resonant azulenoid that consists of four azulenes arranged in the pattern of Figure 4 (where empty rings all hexagons), and embedded in the surface of a torus. A short form of the connection table is shown in Table 2.*

* The expression {x} indicates the largest integer that is not greater than x. For example, {3.8} = 3.

Azulene number	The vertices connected to these positions of each azulene number							
	1	2	4	5	6	7	8	10
0	16	24	22	35	11	37	30	28
1		34	32	25		27	40	38
2	36				31			
3								

Table 2. *An abbreviated form of connection table for the diagram shown in Figure 9.*

Some economies of recorded information may now be effected. Since every azulene is numbered in the same way, the connections of each azulene within itself can be 'taken as read' and recorded as a general property of the encoding scheme. For a system of A azulenes, therefore, we record only $8A$ elements. In the example of Figure 9, there are four azulenes and so $8A=32$ elements. A further small economy is now available. If backward connections (i,j where $i<j$) are ignored, then because all connections outwards from the last azulene will be to vertices with a lower valued label, it follows that the last row of Table 2 will always be empty, so that a single string of $8(A-1)$ elements is sufficient, if it is produced by concatenating all but the last row (24 elements in the case of Table 2).

It is important to remember, as noted above, that in this scheme the set of *azulenes* includes a member that is labelled zero, but that the *vertex* numbers run from one; zeros in the final encoded string represent null connections – empty places in Table 2. For a very large system it is possible to shorten the string a little further by recording, at each new space, not zero, but the number of consecutive empty spaces before the next valid connection. The different significance of this "spacing" number is distinguished by giving it a negative value. The small cost of this operation is to render the length of the stored string unpredictable. However in this, as in all matters of concision mentioned here, the advantages and disadvantages are almost entirely about ease of human recognition and manipulation. In these days of abundant and cheap computer memory, physical storage space as such becomes a significant concern only for very large systems. It is worth pointing out that it is well worthwhile to label such structures in the manner described above, for its clarity, whether or not the possible further compaction mentioned is adopted.

3.3 A special case: fully resonant toroidal azulenoids where every azulene is surrounded by the same pattern of rings, and is connected to no more than six other azulenes.

A method for this particular subset of these networks uses fully resonant benzenoids as geometric templates for classifying them. Toroidal benzenoids in general can be both characterised and enumerated in terms of strings, each of three integers *a*,*b*,*d*. (The last one is called *d* for an historical reason: the code actually derives from a four-element 2x2 matrix, but this can always be chosen in such a way that of the four elements *a,b,c,d*, *c* is zero.[30])

A toroidal benzenoid is fully resonant if the parameters (*a* x *d*) and (*b* + *d*) are both multiples of three, so that this subgroup of the toroidal benzenoids is also well-defined, with one caveat – that the set of full hexagons is not unique until one hexagon is arbitrarily defined as full – although this does not affect the argument used here. Suppose now that we draw an azulene, with a little distortion, and scaled to fit as tightly as possible inside each full hexagon of the biperiodic pattern of the torus. If we now suppress the polyhex grid and label the azulenes, we can draw one or more sets of inter-azulene connections, bearing in mind that, overall, a drawing must be self-consistent, with no crossings. The reason for the limit of six other azulenes, using this method, is now apparent – a full hexagon is spatially surrounded by six other full hexagons in a fully benzenoid sheet.

If the pattern is the same for every azulene, then this can be denoted by some predefined standard alpha-numeric symbol *p*, and the complete structure represented by the four integer code *a*,*b*,*d*,*p*. Furthermore, every possible fully resonant toroidal azulenoid with this pattern can then be enumerated.

If the orientation of azulene and/or the inter-azulene pattern varies throughout the structure, then matters are less simple of course, and there may be no escaping the need to record detailed adjacency information as above (3.2). Even then however, the borrowed *a*,*b*,*d* code may still be a useful parameter to record (because it quickly summarises the global topology), despite the fact that its information content is, strictly, only a repetition of what is implicit within the adjacency matrix.

Another caveat to observe is that, as already noted, azulene is less symmetric than a hexagon. Any toroidal benzenoid, defined by a standard *a*,*b*,*d* code, may have up to six alternative forms (numerical values of *a*,*b*,*d*) that represent different precursor quadrilaterals excised from a graphite sheet, but which are, by symmetry, all equivalent when made into a

torus. When azulenes are superimposed on full hexagons as described, these equivalences of code forms cannot be assumed, and after application of the toroidal benzenoid generator, every output value must be checked for novelty.

3.3.1. An example: toroidal fully resonant azulenoids that have 180 vertices.

Here there must be 18 (180/10) azulenes. If each of these is replaced by a hexagon then we have 18 x 6 = 108 vertices. The first requirement therefore is to enumerate toroidal polyhexes with 108 vertices (and therefore 54 hexagons) in total. (There are 21 such structures of this size, each with either three or six equivalent forms.[31]) As an illustrative example, the particular fully resonant toroidal benzenoid 18-6-3 is shown in Figure 10, and converted to one of the corresponding azulenoids that conform to this arrangement (Figure 11).

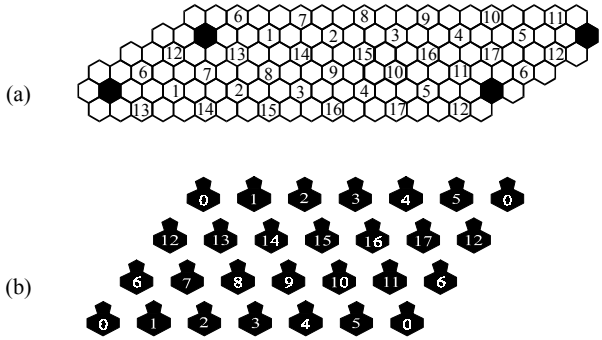


Figure 10. *Using a fully resonant toroidal benzenoid as a template for a fully resonant toroidal azulenoid: (a) A section of the biperiodic pattern for torus 18-6-3 is drawn. Then, starting from 'hexagon-zero' - arbitrarily selected and defined to be 'full' – only the other full hexagons are labelled. (b) All the full hexagons are converted to azulenes and the polyhex grid suppressed.*

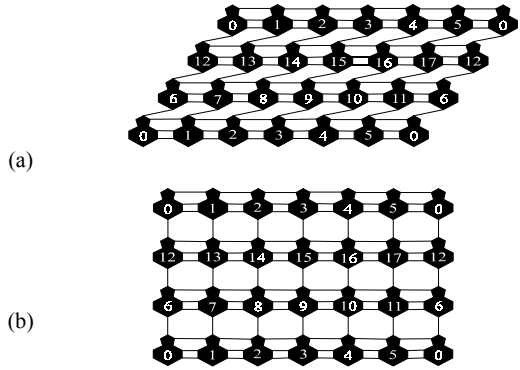


Figure 11. *Converting the biperiodic pattern of* Figure 10(b) *to a connected torus.*
(a) Here the convention that 'east-west' and 'northeast-southwest' represent the two orthogonal directions required for a toroidal embedding is used, and connections for the simple 4-6-8 empty ring pattern are added. (b) The diagram is now rearranged to a less artificial and easier to read form.

CONCLUSION

Although fully resonant azulenoids form a well-defined subset of structures derived from 3-valent networks, the variability of azulene orientation, the variety of possible ring sizes and their distribution pattern forming the empty set means that they are more complicated to deal with than their benzenoid counterparts. Nevertheless, certain toroidal species can be encoded quite simply and, in general, a more informative form of connection table is readily available.

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