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Central vertices versus central rings in polycyclic systems

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This naive supposition that the central vertex(es) in polycyclic graphs should always belong to central ring(s) was examined for various cases of systems containing condensed (fused) 3-, 4-, 5-, 6- and 7-membered rings, as well as combinations of 5- and 7-membered rings. It was found that this conjecture is a general trend valid in the great majority of cases. However, counterexamples with the smallest number of rings are reported for all types of these systems.

1. Introduction

A well-known theorem in graph theory [1] states that acyclic connected graphs (trees) have a unique center, centroid and median consisting of one vertex or a pair of adjacent vertices. The center has the minimax property of having the smallest eccentricity, the centroid has the minimax property of having the smallest weight, and the median has the smallest vertex distance (or distance sum). In trees, the centroid coincides with the median [2,3]. The center and centroid of trees may, or may not, coincide. Examples and definitions may be found in monographs [1,3] and papers [4,5]. Based on the centroid as a graph invariant for trees, Read developed a coding and nomenclature system for acyclic structures [6].

In our previous papers [7–10], we proposed algorithms for restricting the number of central vertices in cyclic graphs, in the hope to attain comparable simplicity to that encountered for trees. Generalized definitions have been advanced in these papers for a graph center, with the aim to approach the "ultimate solution" of the problem by producing central vertices that are topologically equivalent (belonging to the same orbit of the graph automorphism group).

The central rings in benzenoid hydrocarbons became also of interest by being regarded initially as central vertices in the so-called dualist graphs or simply dualists [11,12] (graphs whose vertices represent the central points in the hexagonal benzenoid rings). This idea proved to be a fruitful one, providing a convenient graph-based centric nomenclature and coding of benzenoid hydrocarbons [13]. A similar version of centric benzenoid nomenclature has been proposed lately [14]. The concept of supergraphs was also put forward [15] in which each supergraph vertex represents a ring irrespective of its size. This concept was utilized in developing classification, coding and complexity of linear reaction mechanisms in chemical kinetics [16–18]. Another application is the proposed universal nomenclature and coding of chemical compounds [19] which makes use of central vertices for acyclic structures, central rings for polycyclic structures and even central fragments (in a so-called fragment graph, whose vertices represent molecular fragments) for very complex molecules.

In continuing the series of studies on graph centers in the present paper we try to elucidate another point of importance: the interrelations between the central vertices and central rings in planar connected simple graphs. Graphs containing condensed (fused) 3-, 4-, 5-, 6- and 7-membered rings are discussed with this purpose.

2. Some definitions

The classical definition of the graph center was put forward by several well-known mathematicians in the 19th century (Jordan, Sylvester, Cayley) [20,21]. It makes use of distances in graphs. The distance d_{ij} between vertices i and j is an integer specifying the number of graph edges separating the two vertices along the shortest path between them. The largest distance from a vertex i to any other vertex in the graph is called vertex eccentricity, e_i. The vertices with minimal eccentricity are called central, or, in other words, central are those vertices i which satisfy the minimax criterion

$$e_i = \max d_{ij} = \min \; . \tag{1}$$

The concept of a graph center has initially been defined for acyclic graphs (trees) for which it specifies a single central vertex or a bicenter, i.e. two adjacent vertices which are endpoints of a central edge.

Another centric concept developed for such graphs is that of centroids or mass centers. It is based on the idea of weighting each of the tree vertices. All branches, $1, 2, \ldots, k, \ldots$ originating from a certain vertex i are taken into consideration and the number of edges N_{ik} they contain is counted. The largest one defines the vertex weight, w_i. Hence, the centroid (mass center) is (are) the graph vertex(es) having the minimal weight, according to the minimax condition

$$w_i = \max N_{ik} = \min \; . \tag{2}$$

A third concept introduces the graph median as vertex(es) having the minimal vertex distance, d_i. The latter is also called vertex status or distance sum because it represents the sum of the distances from a certain vertex i to all other graph vertices. Once again, this type of graph center is determined as being the "closest" to the remaining vertices,

$$d_i = \sum_j d_{ij} = \min \, , \tag{3}$$

where i is the graph median.

Both the classical graph center and the graph median are applicable to acyclic, as well as to cyclic, graphs. However, in the latter case they frequently qualify as central a rather large number of graph vertices, and even, in some extreme cases, all graph vertices possess this property. This was what prompted the extension and generalization of the graph center definitions in a series of our previous publications [7–10]. They will not be presented here because in a first study on the interrelation between the central vertices and central rings in graphs one necessarily has to limit one's efforts to the simplest and best known kinds of graph centers – the classical center and the median.

3. Benzenoids

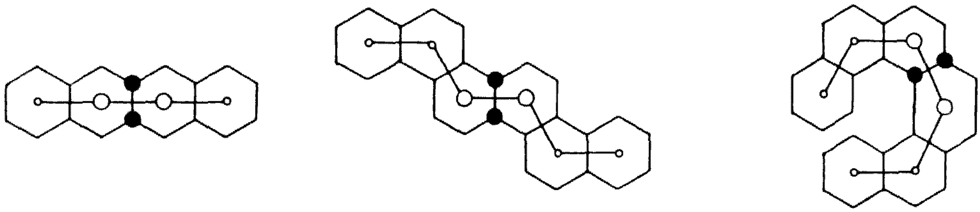
We shall use the term *benzenoid* or *polyhex* [22] for indicating polycyclic systems formed from six-membered rings. Hydrogen-depleted graphs will be used throughout. No restrictions exist as to the geometrical (as distinct from graph-theoretical) planarity of such systems, therefore benzenoids will include compounds such as [6] helicene (their graphs, however, are always planar).

The *dualist* of a benzenoid [11] consists of vertices which are the centers of hexagons, and of edges connecting vertices that correspond to condensed hexagons, i.e. to hexagons sharing an edge. When the dualist is acyclic, the benzenoid is called cata-condensed (*catafusene*); when it has three-membered rings, the benzenoid is called peri- condensed (*perifusene*); when it has larger rings which are not peripheries of three-membered ring aggregates, the benzenoid is called corona-condensed (*coronoid*).

3.1. NONBRANCHED CATAFUSENES

The dualist of a nonbranched catafusene is a string of vertices with degrees 1 and 2, whose center is one vertex or a pair of adjacent vertices. The corresponding benzenoid rings are therefore called central rings. In most cases, the central vertices of the benzenoid (symbolizing carbon atoms) belong to the central rings of the benzenoid hydrogen-depleted graph. Thus, in an acene, e.g. graph **1**, or a fibonacene (zig-zag catafusene) e.g. graph **2**, both with $2k$ benzenoid rings, the center of the dualist is a pair of adjacent vertices, and the central vertices of the benzenoid consist in the shared vertex pair crossing the center of the dualist, i.e. these are the vertices on the edge shared by the two central rings. The same rule applies to a helicene with $2k$ benzenoid rings, e.g. **3**, which is isomeric and isoarithmic with a fibonacene having the same number $2k$ of benzenoid rings (fig. 1). Two benzenoids are called isoarithmic if they have the same number of Kekule structures.

Proceeding from numerous examples one is tempted to conjecture as a general result that the central vertices always belong to the central rings. However, this is

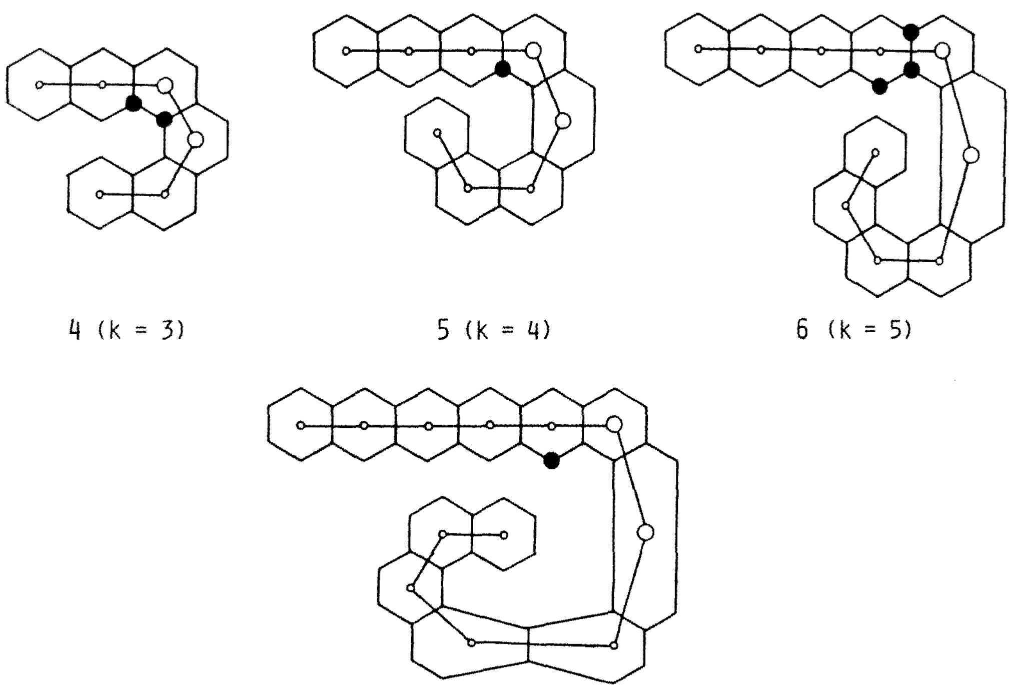


1 (k = 2) 2 (k = 3) 3 (k = 3)

Fig. 1. Nonbranched catafusenes **1**– **3** with their dualists, whose vertices are open circles; the larger open circles indicate the center or bicenter of the dualist; the central vertices of the benzenoid are indicated by black points.

not always true, and in the following we present counterexamples containing the smallest benzenoid hydrocarbons in which the central vertices do not belong to the central rings.

Let a nonbranched catafusene be composed of $2k$ benzenoid rings, k of which are linearly condensed (acene-like), and the remaining k rings are helicenic. The first such systems **4**–**7** are presented in fig. 2.



4 (k = 3) 5 (k = 4) 6 (k = 5)

7 (k = 6)

Fig. 2. A series of nonbranched catafusenes **4**–**7** with dualists and central vertices, indicated as in fig. 1, in which the higher members do not have the central vertex(es) in the central rings.

It is easy to prove that: (i) **4** is the smallest nonbranched catafusene with $2k$ rings in which one of the central vertices does not lie on the common edge between the two central rings, but still the central vertices belong to the central rings; (ii) **5** is the smallest nonbranched catafusene with $2k$ rings in which no central vertex lies on the shared edge between the two central rings, but still the central vertices belong to the central rings; (iii) **6** is the smallest nonbranched catafusene with $2k$ rings in which one of the central vertices does not belong to any of the central rings; (iv) **7** is the smallest nonbranched catafusene with $2k$ rings in which none of the central vertices belongs to any of the central rings.

If the total number of rings is odd ($2k + 1$), the benzenoid will have a single central ring and the smallest nonbranched catafusenes with the above properties (iii) and (iv) will have three rings less.

3.2. BRANCHED CATAFUSENES

Again the dualist in this case is a tree, therefore it has a uniquely defined centroid coinciding with the median, as well as a uniquely defined center. Thus, these benzenoids have either a central ring, or a pair of condensed central rings. The obvious inference is that in most cases the central vertices of these benzenoids will belong to the central ring or rings.

Fig. 3 contains an example **8** whose dualist has a vertex (**A**) as both its center and centroid. By the distance sum criterion, vertex 1 is the median of the benzenoid, and by the eccentricity criterion vertex 2 is its center, satisfying indeed the above inference.

A series of branched catafusenes whose central vertices always belong to the central ring is presented in fig. 4. Starting with dualists whose last endpoint is **C**, the central vertices are the three indicated by black points of the central ring in **9**. For **10**, when the dualist has its endpoint **C**, vertex 2 is the center of the polyhex, but for all higher members of this series, vertices 1 and 2 are the centers.

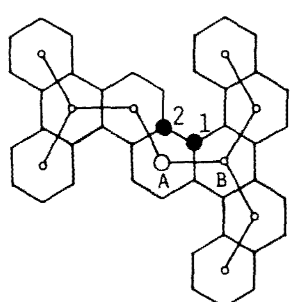


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Fig. 3. A branched catafusene **8** with its dualist (see fig. 1 for further conventions).

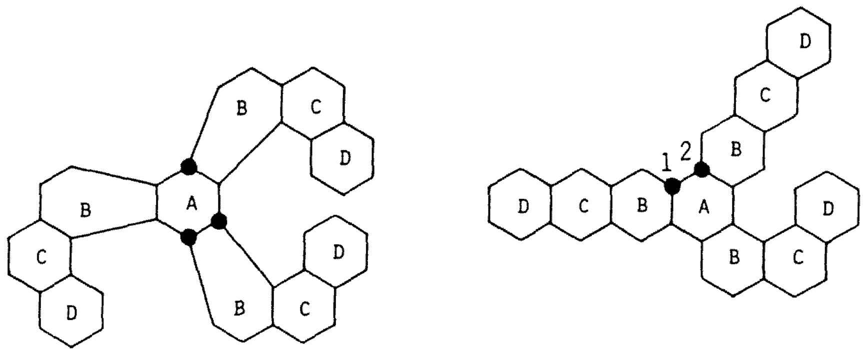

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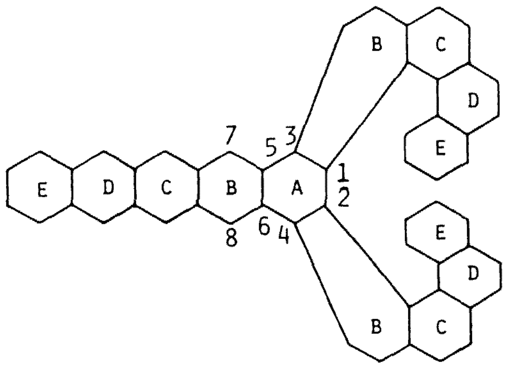
Fig. 4. Two series of branched catafusenes (**9**, **10**) with their dualists, central ring (**A**) and central vertices (black points).

We now proceed to find systems which contradict the above inference. Figure 5 and table 1 present three such series, with the indicated central ring **A** having three equally long branches. In the polyhexes **11** and **12** with bilateral symmetry, the systems with $r = 4$, 7 and 10 benzenoid rings have their central vertices belonging to the uniquely defined central ring **A**. The smallest benzenoid in series **11** whose central vertices (a nonadjacent pair) do not belong to the central ring has $r = 19$ rings, whereas in series **12** it has only 16 rings. Also for the asymmetric series **13**, the smallest such benzenoid has 16 rings.

3.3. PERIFUSENES

Subdivisions in this category include Kekulean perifusenes and non-Kekulean ones. The latter can be obvious (with an excess of starred over nonstarred vertices, to adopt the Longuet–Higgins terminology for bipartite graphs), e.g. **14**, or concealed (having equal numbers of starred and nonstarred vertices, yet having no Kekule structure, or no perfect matching), e.g. **15**. Necessary and sufficient criteria for perifusenes to be concealed non-Kekuleans were found recently [23–27]. With perifusenes, the center, centroid, and median of the dualist will be defined by the criteria (1)–(3) presented in section 2.

Graph **14** in fig. 6 shows a series of obvious non-Kekulean perifusenes in which only the first members have central vertices belonging to the three central rings. The structure with 11 rings is the last one in which this is still true (vertices 2 and 3) but it is also the first structure in the series in which a vertex not belonging to the



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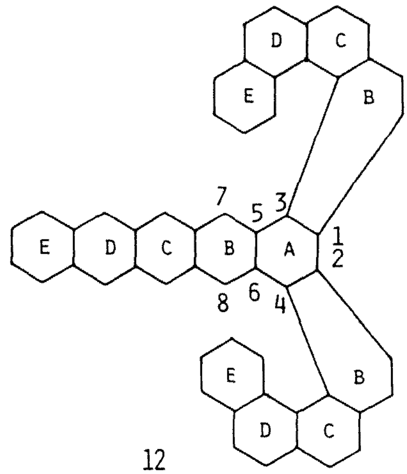

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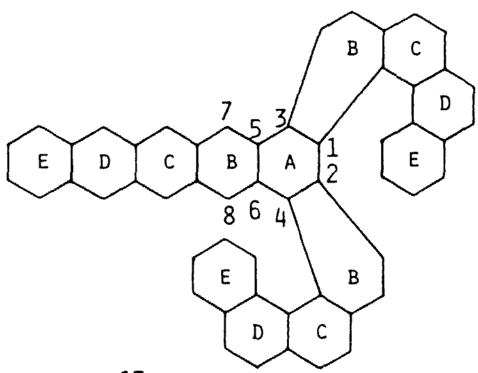

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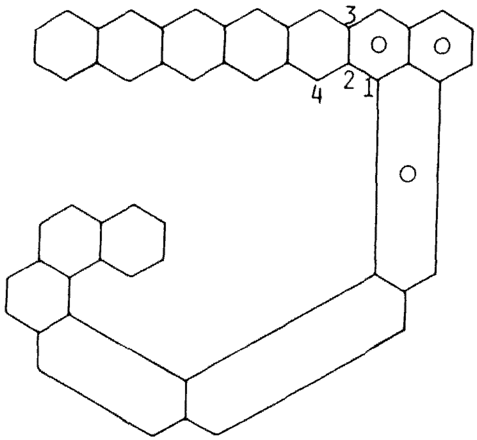
Fig. 5. Three series of branched catafusenes (**11–13**) whose central vertices no longer lie on the central ring **A** in the higher members of the series.

Table 1
Central vertices of the branched catafusenes **11–13** from fig. 5 whose endpoints of the dualists are denoted by the indicated letter.

Benzenoid	B	C	D	E	–	–
Rings (r)	4	7	10	13	16	19
11	1–6	3, 4	3–6	5, 6	5–8	7, 8
12	1–6	5, 6	5, 6	5–8	7, 8	7, 8
13	1–6	4, 5	5	5–7	7	7, 8



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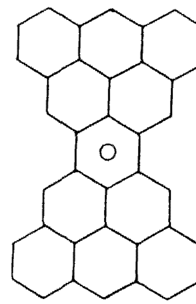

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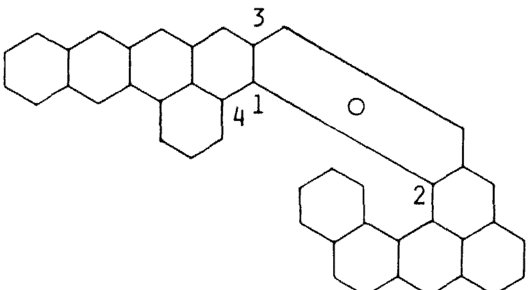

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Fig. 6. Three cases of perifusenes: obvious non-Kekulean (graph **14**), concealed non-Kekulean (graph **15**) and Kekulean (graph **16**). In the higher members of series **14** and **16** (having 11 and 13 rings, respectively) the single central vertex 4 does not belong to the central ring(s).

central rings is a central one (vertex 4). The structure with 13 rings has no more central vertices belonging to the central rings; the single center is vertex 4. Likewise, graph **16** in fig. 6 presents a series of Kekulean perifusenes with fixed double bounds along the edges of the six-membered rings which are drawn in elongated form. This is a series in which the inference for an interrelation between central vertices and rings is violated as early as in the perifusene with 9 rings where one of the central vertices (vertex 4) does not belong to the central ring. In the next member of the series having 11 rings the single central vertex 4 does not belong to any of the central rings. The concealed non-Kekulean perifusenes are exemplified in fig. 6 with a single structure in which the six central vertices all belong to the central ring.

Figures 7 and 8 present examples of Kekulean perifusenes forming series in which again the first members have the central vertices of the benzenoids belonging to the central rings, but for the higher members this is no longer true. We examine systems having pyrene and perylene units at the graph center. Figure 7 and table 2 describe two series, **17** and **18**, based on pyrene. In both cases, the systems with 12 rings are the smallest ones with one central vertex not belonging to the central rings, and the systems with 14 rings are the smallest ones with no central vertices belonging to the central rings.

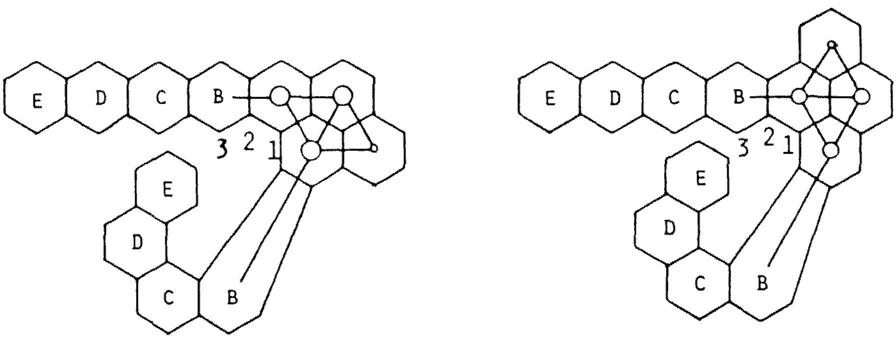

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Fig. 7. Two series (**17**, **18**) of Kekulean perifusenes based on pyrene in the higher members of which the central vertices (e.g. vertex 3) lie outside the central rings indicated by larger open circles.

Table 2
Central vertices of the two Kekulean perifusene series **17** and **18** based on pyrene from fig. 7 whose endpoints of the dualists are denoted by the indicated letter.

Benzenoid	B	C	D	E	–
r	6	8	10	12	14
17	1	1, 2	2	2, 3	3
18	1, 2	1, 2	2	2, 3	3

In fig. 8 and table 3 are shown two series based on perylene. The smallest member of series **19** whose central vertex does not belong to the central ring has 13 rings, and the smallest member whose central vertex does not belong to the perylene subgraph has 17 rings. The corresponding smallest members of series **20** have 11 and 19 rings, respectively. Thus, the smallest Kekulean benzenoid hydrocarbon in which none of the central vertices belongs to a central rings is that with 11 rings in series **20**.

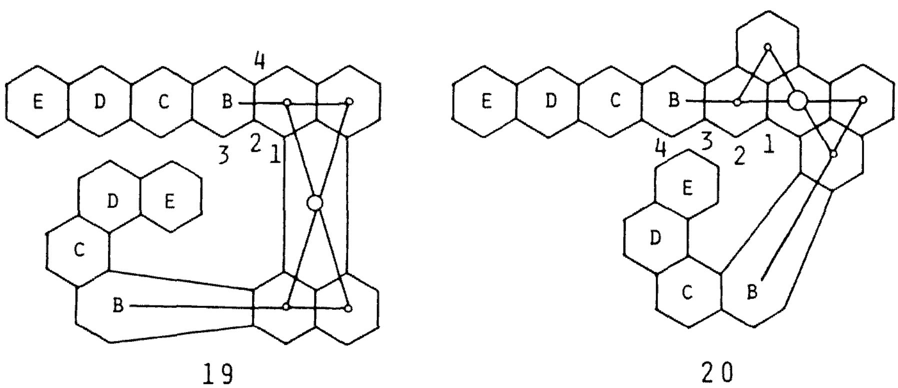

Fig. 8. Two series (19, 20) of Kekulean perifusenes based on perylene whose higher members have the central vertices (e.g. 3,4) not belonging to the central ring indicated by the larger circle.

Table 3
Central vertices of the two Kekulean perifusene series (**19** and **20**) based on perylene from fig. 8 whose endpoints of the dualists are denoted by the indicated letter.

Benzenoid	B	C	D	E	–	–	–
r	7	9	11	13	15	17	19
19	–	1	1, 2	2	2, 3	3	3, 4
20	1	1, 2	2	2, 3	3	3, 4	4

4. Nonbenzenoid polycyclic condensed systems

We shall discuss, for the sake of mathematical completeness, chemically irrelevant systems composed either only of 4- or only of 3-membered rings. As it is well known, the plane can be covered only by lattices of regular 3-, 4- and 6-gons; we have already discussed the hexagons in the previous section. The three above lattices gave rise to the still unsolved graph- theoretical problems of the "animal cells in triangular, square, and hexagonal animals", problems widely discussed by Harary [1]. Then, we shall discuss chemically relevant non-benzenoid condensed polycyclics composed of 5- and 7-membered rings.

4.1. "SQUARE ANIMALS"

We shall examine only 4-membered ring analogs of nonbranched cata-condensed systems, considering again that usually the central vertices will belong to the central rings, but sometimes the topology will lead to exceptions. Such a case is presented in fig. 9 and table 4.

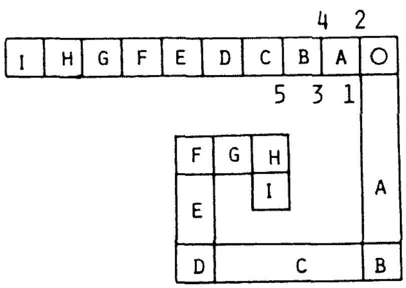

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Fig. 9. A series of nonbranched tetragonal systems (**21**) the higher members of which have their central vertices (e.g. 3,4) outside the central ring indicated by the circle.

Table 4
Central vertices of the series of nonbranched tetragonal systems **21** from fig. 9 whose endpoints of the dualists are denoted by the indicated letter.

Systems	A	B	C	D	E	F	G	H	I
r	3	5	7	9	11	13	15	17	19
centers	1	1	1–3	1–3	3	3	3–5	3–5	5

It may be seen that the smallest member of the series **21** whose central vertices include a point not belonging to the central ring has 7 rings, and that the smallest member of the series which has no central vertex belonging to the central ring has 11 rings.

4.2. "TRIANGULAR ANIMALS"

The analogous problem for systems **22** composed of triangles is shown in fig. 10 and table 5.

An interesting oscillating behavior is observed. The smallest system in this series including among the central vertices a point which does not belong to the central ring has 11 rings; the smallest member of this series which has no central vertex belonging to the central ring has 19 rings.

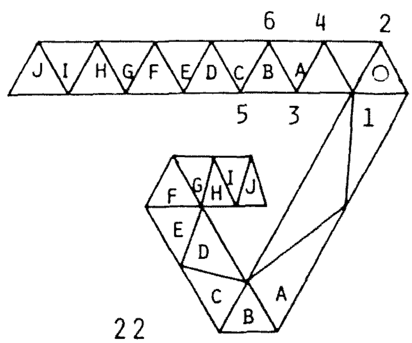

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Fig. 10. A series of nonbranched trigonal systems (**22**) the higher members of which have their central vertices (e.g. 3, 4) outside the central ring indicated by the circle.

Table 5
Central vertices of the series of nonbranched trigonal systems **22** from fig. 10 whose endpoints of the dualists are denoted by the indicated letter.

Systems	A	B	C	D	E	F	G	H	I	J
r	9	11	13	15	17	19	21	23	25	27
centers	1	1–4	1, 3, 4	1–4	1, 3, 4	3, 4	3	3, 4	3	3–6

4.3. NONBRANCHED CATA-CONDENSED SYSTEMS COMPOSED OF 5- MEMBERED RINGS

Analogously to the foregoing systems, fig. 11 and table 6 describe a chain **23** with $2k$ five-membered rings arranged linearly on one side and curved (spiralling) on the other side.

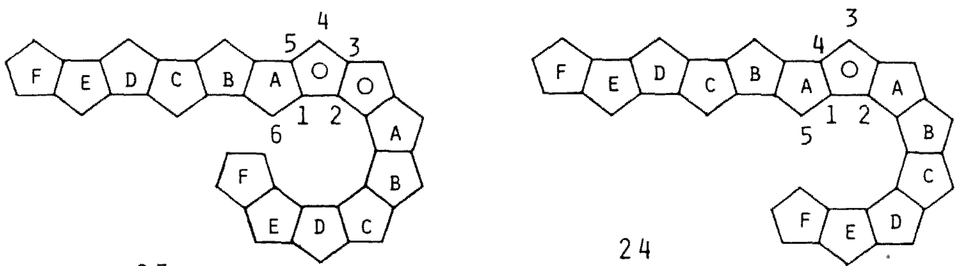

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Fig. 11. Two series of nonbranched cata-condensed systems composed of 5-membered rings: series **23** with even number of rings, whose higher members have central vertices (e.g. 6, 7) outside the pair of central rings indicated by the circles and series **24** with odd number of rings whose higher members have central vertices (e.g. 5, 6) outside the unique central ring.

Table 6
Central vertices of the series of nonbranched cata-condensed systems **23** composed of an even number of 5-membered rings given in fig. 11 whose endpoints of the dualists are denoted by the indicated letters.

Systems	A	B	C	D	E	F	–	–	–
r	4	6	8	10	12	14	16	18	20
centers	2	1–3	1, 2	1	1	1, 4–6	1, 4–6	5, 6	6

Table 7
Central vertices of the series **24** of nonbranched cata-condensed systems composed of odd number of 5-membered rings given in fig. 11 whose endpoints of the dualists are denoted by the indicated letters.

Systems	A	B	C	D	E	F	G
r	3	5	7	9	11	13	15
centers	1–3	1	1	1, 3–5	1, 4, 5	4, 5	5

One can observe that the smallest member of this series including among its central vertices a point which does not belong to the central rings has 14 rings, and the smallest member which has no central vertex belonging to the central rings has 20 rings.

When the number of five-membered rings is odd ($2k+1$), as in series **24**, fig. 11 and table 7, a similar type of fusion leads to the smallest member of the series whose center includes a vertex not belonging to the unique central ring when $2k+1=9$, whereas the smallest member which has no central vertex belonging to the central ring has $2k+1=15$ rings.

4.4. NONBRANCED CATA-CONDENSED SYSTEMS COMPOSED OF 7-MEMBERED RINGS

There exist two possibilities for condensing analogously $2k$ seven-membered rings, giving rise to two series **25** and **26**, as seen in fig. 12.

The smallest member of series **25** (table 8) whose central vertices include a point which does not lie on one of the two central rings, and at the same time no point of the central ring is a central vertex has, 12 rings.

In series **26** (table 9) the interrelation of the central rings and central vertices is violated at considerably smaller systems. Thus, the smallest nonbranched cata-condensed system whose central vertices include a vertex not belonging to the central

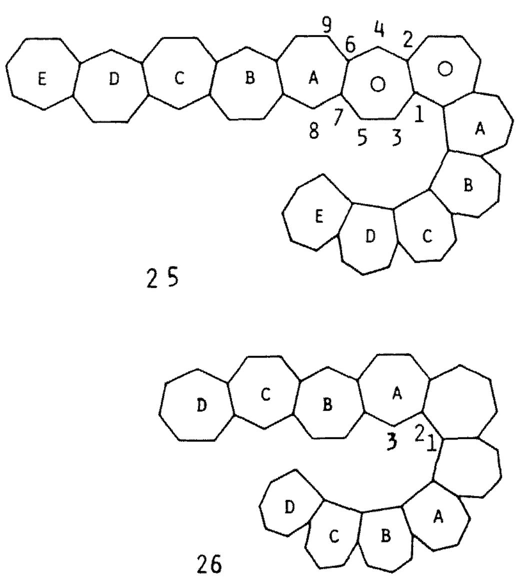

Fig. 12. Two series of nonbranched cata-condensed systems (**25** and **26**) composed of an even number of 7-membered rings, the higher members of which have central vertices outside the pair of central rings indicated by the circles.

ring has 8 rings, whereas the smallest similar system in which no central vertex belongs to a central ring is that with only 10 rings. The comparison of series **25** and **26** and the corresponding tables shows the importance of both the ring size and the topology of ring fusion.

Table 8
Central vertices of the series of nonbranched cata- condensed systems **25** composed of an even number of 7-membered rings (fig. 12) whose terminal rings are denoted by the indicated letters.

Systems	–	A	B	C	D	E
r	2	4	6	8	10	12
centers	1, 2	2, 3	3–5	4–7	7	8, 9

Table 9
Central vertices of the series **26** of nonbranched cata-condensed systems (fig. 12) composed of an even number of 7-membered rings whose terminal rings are denoted by the indicated letters.

Systems	A	B	C	D
r	4	6	8	10
centers	1	1, 2	2, 3	3

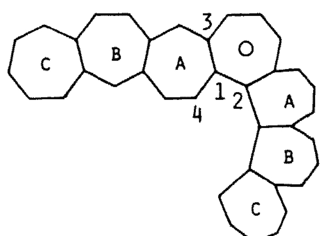

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Fig. 13. A series of nonbranched cata-condensed systems (**27**) composed of an odd number of 7-membered rings, whose higher members have central vertices not belonging to the unique central ring indicated by a circle.

Table 10
Central vertices of the series **27** of nonbranched cata-condensed systems (fig. 13) composed of an odd number of 7-membered rings whose terminal rings are denoted by the indicated letters.

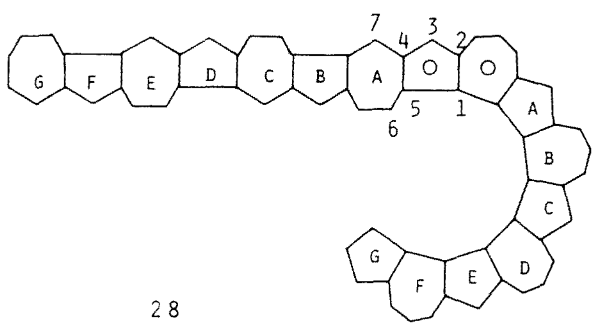
Systems	A	B	C
r	3	5	7
centers	1, 2	1, 3, 4	4

When the number of seven-membered rings is odd ($2k+1$), from the two possibilities similar to the series **25** and **26**, the one analogous to **25**, namely series **27** (fig. 13 and table 10) leads to the smaller graphs with central vertices off the central rings: the smallest member of the series whose central vertices include a vertex not belonging to the unique central ring has only five rings, while the smallest member of the series with no central vertex belonging to the central ring has seven rings.

4.5. CATA-CONDENSED NONBRANCHED SYSTEMS WITH $2k$ ALTERNATING 5- AND 7-MEMBERED RINGS

Analogously to the previous cases, starting from azulene which is the smallest representative of this class, we investigated the series **28** shown in fig. 14 and table 11.

The smallest system in this series having among its central points a vertex which does not belong to the central rings has 10 rings, and the smallest system with no central vertex belonging to the central ring has 16 rings. Of course, there are many



28

Fig. 14. A series of nonbranched cata-condensed systems **28** with alternating 5- and 7-membered rings. The members having at least 12 rings have central vertices outside the pair of central rings indicated by the circles.

Table 11
Central vertices of the series of nonbranched cata- condensed systems **28** composed of $2k$ alternating 5- and 7-membered rings given in fig. 14 whose terminal rings are denoted by the indicated letters.

Systems	A	B	C	D	E	F	G	–
r	4	6	8	10	12	14	16	18
centers	1, 5	1	5	3–6	4, 6, 7	4, 6, 7	7	7

more alternative ways of having nonbranched or branched cata-condensed systems with alternating 5- and/or 7-membered rings (or systems with 5-, 6- and 7-membered rings), but here we examined only the salient, most relevant cases.

5. Concluding remarks

In the foregoing we have reported the main results of a first study on the interrelation of central vertices and central rings in polycyclic simple connected graphs. Most of these graphs contain 6-, 5- or/and 7-membered rings and have vertices with degrees 2 and 3, therefore they correspond to conjugated molecules. The hexagonal systems which have numerous analogs in benzenoid hydrocarbons have been analyzed in more detail by treating cata- and peri-condensed cases, as well as nonbranched and branched ones. In addition, systems with 3- or 4-membered rings with very limited chemical relevance were taken into consideration for the sake of mathematical completeness. Besides theoretical interest these studies could be of use for nomenclature and coding purposes, because shell description or shell coding around a central graph vertex or central atomic rings seem to be a very efficient organizing principle [13–19]. Another area of potential application could be the search for similarity in molecular properties for systems having similar centric atomic or ring patterns.

The most natural interrelation between the central vertices and central rings is the one in which the central vertices belong to central rings, and this was found to occur in the great majority of cases. However, series of strongly asymmetrically fused graphs have been constructed that provide counterexamples to this inference. These are graphs containing a ribbon of cycles half of which are linearly condensed while the other half is maximally curved, i.e. the latter rings are helically arranged. When increasing the size of such a graph by attaching each time a ring on each of its two ends, one attains a fast displacement of the central vertices out of the central rings of the graph. We conjecture that the counterexamples produced in this way are those with the smallest possible number of rings for each type of cyclic graph under consideration. Indeed, this statement may be regarded as a challenge for further investigations. However, the major question which still needs to be answered is a much more general one: to what extent do symmetry and topology control the interrelation of the central vertices and rings in graphs? We hope to report more results on the matter in the near future [28].

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