

Connected Components of Resonance Graphs of Carbon Nanotubes

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Abstract

Carbon nanotubes are chemical compounds made of carbon which possess a cylindrical structure. Open-ended single-walled carbon nanotubes are called tubulenes. The resonance graph of a tubulene reflects the interference among its Kekulé structures. Our work is motivated by [15] where some basic properties of resonance graphs of benzenoid systems were investigated.

In the present paper it is shown that every connected component of the resonance graph of a tubulene is either a path or a graph of girth 4. The example for the construction of an arbitrary path as a connected component of the resonance graph is given. We also provide a condition for a tubulene under which every connected component of its resonance graph different from a path without vertices of degree one is 2-connected.

1 Introduction

Benzenoid graphs are 2-connected planar graphs such that every inner face is a hexagon. Benzenoid graphs are generalization of *benzenoid systems*, also called *hexagonal systems*, which can be defined as benzenoid graphs that are also subgraphs of a hexagonal lattice (for details see [5, 6]).

If we embed benzenoid systems on a surface of a cylinder and join some edges we obtain structures called open-ended single-walled carbon nanotubes also called tubulenes (note that there are also closed-ended single-walled carbon nanotubes i.e. carbon nanotubes with caps). Carbon nanotubes are carbon compounds with a cylindrical structure. The extremely large ratio of length to diameter causes unusual properties of these molecules, which are valuable for nanotechnology, electronics, optics and other fields of materials science and technology. Nanotubes were observed in 1991 [7] in the carbon soot of graphite electrodes during an arc discharge. The first macroscopic production of carbon nanotubes was made in 1992 by two researchers at NEC's Fundamental Research Laboratory [2]. In 1996 Smalley group at Rice university successfully synthesized the aligned closed-ends single-walled carbon nanotubes [11]. Nanotubes are members of the fullerenes, i.e. carbon molecules in different shapes such as sphere, ellipsoid, tube, which may also contain pentagonal rings.

The *resonance graph* $R(G)$ of a benzenoid system or a tubulene G reflects the structure of perfect matchings of G . The concept of the resonance graph was introduced independently in mathematics (under the name Z -transformation graphs) by Zhang, Guo, and Chen [15] and in chemistry first by Gründler [4] and later by El-Basil [3] as well as by Randić with co-workers [8, 9]. The definition is quite natural and has a chemical meaning since perfect matchings of G are Kekulé structures of a corresponding hydrocarbon molecule. Some basic properties of resonance graph of benzenoid systems can be found in [14].

Resonance graphs of some families of tubulenes were considered in [17, 18, 19] and in [1] the equality of the Zhang-Zhang polynomial of a spherical benzenoid system and the cube polynomial of its resonance graph was shown. It was shown in [12] that the resonance graph of every tubulene is always bipartite. Also, a condition under which the resonance graph of a tubulene is not connected was given.

In [15] the authors proved that the resonance graph of any benzenoid system is either a path or a graph of girth 4. It was also shown that in the last case the resonance graph without vertices of degree one is 2-connected. In this paper we generalize these results to tubulenes. Some ideas from [15] can be used but the cylindrical structure of tubulenes makes significant differences.

2 Preliminaries

First we will formally define open-ended carbon nanotubes, also called *tubulenes* ([10]). Choose any lattice point in the hexagonal lattice as the origin O . Let \vec{a}_1 and \vec{a}_2 be the two basic lattice vectors. Choose a vector $\vec{OA} = n\vec{a}_1 + m\vec{a}_2$ such that n and m are two integers and $|n| + |m| > 1$, $nm \neq -1$. Draw two straight lines L_1 and L_2 passing through O and A perpendicular to OA , respectively. By rolling up the hexagonal strip between L_1 and L_2 and gluing L_1 and L_2 such that A and O superimpose, we can obtain a hexagonal tessellation \mathcal{HT} of the cylinder. L_1 and L_2 indicate the direction of the axis of the cylinder. Using the terminology of graph theory, a *tubulene* T is defined to be the finite graph induced by all the hexagons of \mathcal{HT} that lie between c_1 and c_2 , where c_1 and c_2 are two vertex-disjoint cycles of \mathcal{HT} encircling the axis of the cylinder. The vector \vec{OA} is called the *chiral vector* of T and the cycles c_1 and c_2 are the two open-ends of T .

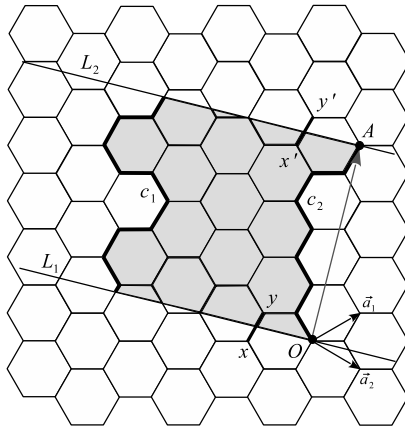


Figure 1: Illustration of a $(4, -3)$ -type tubulene.

For any tubulene T , if its chiral vector is $n\vec{a}_1 + m\vec{a}_2$, T will be called an (n, m) -type tubulene, see Figure 1. Graph G is a *spherical benzenoid system* if G is either a benzenoid system or a tubulene [1].

An *1-factor* of a graph G is a spanning subgraph of G such that every vertex has degree one. Edges of the 1-factor form an independent set of edges i.e. a *perfect matching* of G (in the chemical literature these are known as Kekulé structures; for more details see

[6]). Let G be a spherical benzenoid system and M a perfect matching of G . A hexagon h of G is M -alternating if the edges of h appear alternately in and off the perfect matching M . Such hexagon h is also called a *sextet*. Let G be any graph. An edge of G is *allowed* if it lies in some perfect matching of G and *forbidden* otherwise. A graph G is called *elementary* if it is connected and every edge of G is allowed.

The *resonance graph* $R(G)$ of a spherical benzenoid system G is the graph whose vertices are the perfect matchings of G , and two perfect matchings are adjacent whenever their symmetric difference forms a set of edges of some hexagon of G .

The concept of resonance graph can be extended to any plane bipartite graph (see [13]). Let G be a plane bipartite graph and M a perfect matching of G . A cycle C in G is M -alternating if the edges of C appear alternately in and off the M . The vertices of G can be colored white and black so that adjacent vertices receive different colors. Then an M -alternating cycle C of G is said to be *proper* if every edge in $E(C) \cap M$ goes from white end-vertex to black end-vertex along the clockwise orientation of C . Let $F_0(G)$ denotes the set of all inner faces of G and $F(G)$ the set of all faces of G . Let $F \subset F(G)$. Then the *restricted resonance digraph* of G , denoted by $\vec{R}_F(G)$, is the digraph whose vertices are the perfect matchings of G such that there exists an arc from M_1 to M_2 if and only if the symmetric difference $M_1 \oplus M_2$ is a proper M_1 -alternating cycle that is the boundary of a face f in F . Neglecting all directions of arcs of $\vec{R}_F(G)$ we get the *restricted resonance graph* $R_F(G)$.

Let G be a connected graph and $v \in V(G)$. Then v is a *cut vertex* if its removal disconnects G . A connected graph is *2-connected* if it does not contain a cut vertex.

The *Cartesian product* $G \square H$ of graphs G and H is the graph with the vertex set $V(G) \times V(H)$ and $(a, x)(b, y) \in E(G \square H)$ whenever $ab \in E(G)$ and $x = y$, or, if $a = b$ and $xy \in E(H)$.

3 Some results about resonance graphs of tubulenes

In this section we prove some properties of resonance graphs of tubulenes. It is shown that every connected component of the resonance graph is either a path or a graph of girth 4. Note that if a directed graph can be represented as a distributive lattice this

property follows immediately. In [13] it was proved that if G is a plane elementary bipartite graph and $F \subset F_0(G)$ then each connected component of the directed resonance graph of G restricted to F can be represented as a distributive lattice, but tubulenes are not elementary graphs. Further it was shown in the same paper, that if G is a plane bipartite graph then each connected component of the directed resonance graph can be represented as a distributive lattice (without any restriction on $F_0(G)$). Since one open-end of a tubulene T is an inner face in every planar drawing of T the last result can not be used in our case either.

We also provide a condition for a tubulene such that if some connected component of its resonance graph is not a path, then this component without vertices of degree one is 2-connected. Some examples of tubulenes such that its resonance graph contains a path P_n as a connected component are also given.

Lemma 3.1 *Let T be a tubulene with a perfect matching and H a connected component of the resonance graph $R(T)$ such that H is not a path. If $V_1(H)$ is the set of all vertices in H that have degree one and $M \in V(H) - V_1(H)$, then we can find in a tubulene T at least two disjoint hexagons which are M -alternating cycles.*

Proof. Let $M \in V(H) - V_1(H)$. We must show that we can find in a tubulene T at least two disjoint hexagons which are M -alternating cycles. Consider two options:

1. If M has degree more than two in H we can find three hexagons h_1, h_2 and h_3 of T which are M -alternating cycles. If every two of them have an edge in common we get a situation in Figure 2. This is a contradiction since a graph in the figure does not have a perfect matching. Thus, at least two of the hexagons h_1, h_2 and h_3 are disjoint.

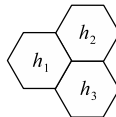


Figure 2: Position of hexagons h_1, h_2 and h_3 in case 1. which is not possible.

2. If M has degree two in H then there are only two M -alternating cycles which are hexagons of T . Let h_1 and h_2 be these hexagons. If h_1 and h_2 are disjoint, the proof is obvious. So suppose that h_1 and h_2 have an edge in common.

Let $M_1 = M \oplus E(h_2)$ and $M'_1 = M \oplus E(h_1)$. Obviously, any M_1 -alternating hexagon of T , which is not h_2 , must have a common edge with h_2 since otherwise there are more than two hexagons which are M -alternating cycles. In Figure 3 we can see

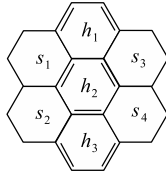


Figure 3: Perfect matching M_1 .

that hexagons h_1, s_1, s_2, s_3, s_4 can not be M_1 -alternating. Hence, there can be at most one hexagon besides h_1 , say h_3 , which is an M_1 -alternating cycle. Similar is true for M'_1 , i. e. there is at most one hexagon besides h_1 , say h'_2 , which is an M'_1 alternating cycle. Hence, vertices M_1 and M'_1 have both degree at most two in H . We can repeat this procedure to get linearly connected hexagons h_2, h_3, h_4, \dots and h_1, h'_2, h'_3, \dots . Since they lie on a tubulene it could happen that two of them are

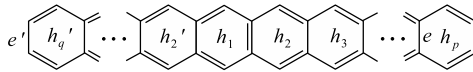


Figure 4: Perfect matching M .

equal, say h_p and h'_q (see Figure 4). In that case edges e and e' coincide but then M is not a perfect matching. Therefore all hexagons are different and since T is finite, with repeating the above procedure we get a path $M'_r M'_{r-1} \dots M'_1 M M_1 \dots M_{t-1} M_t$ ($r \geq 1, t \geq 1$), which is a connected component of H . Since H is connected, H must be a path itself and this is a contradiction. Therefore, hexagons h_1 and h_2 are disjoint.

We have proved that in a tubulene T there are two disjoint hexagons h_1 and h_2 which are M -alternating cycles. The proof is complete. ■

With Lemma 3.1 we can prove the following theorem.

Theorem 3.2 *Let T be a tubulene with a perfect matching and H a connected component of the resonance graph $R(T)$. Then H is either a path or a graph of girth 4.*

Proof. Suppose that H is not a path. We will see that in this case H must be a graph of girth 4. The set of all vertices in $V(H)$ which have degree one will be denoted by $V_1(H)$. If the set $V(H) - V_1(H)$ is empty it follows that H is the path P_2 , which is a contradiction since H is not a path. Hence, let $M \in V(H) - V_1(H)$.

By Lemma 3.1, in a tubulene T there are two disjoint hexagons h_1 and h_2 which are M -alternating cycles. Thus, M lies in a 4-cycle $MM_1M_2M_3$ where $M_1 = M \oplus E(h_1)$, $M_2 = M_1 \oplus E(h_2)$ and $M_3 = M_2 \oplus E(h_1)$. By Theorem 3.2 in [12] the resonance graph $R(T)$ is bipartite, therefore, H is bipartite too. Since every vertex lies in some 4-cycle, the girth of H is 4 and the proof is completed. ■

Theorem 3.2 says that every connected component of a resonance graph $R(T)$ is either a path or a graph of girth 4. But it is not so easy to find an example of a tubulene T such that its resonance graph $R(T)$ has a connected component which is a path. Hence, we state the following theorem.

Proposition 3.3 *Let n be a positive integer. Then there is a tubulene T such that the resonance graph $R(T)$ has a connected component which is isomorphic to a path P_n .*

Proof.

1. If $n = 1$ the proof is obvious since we know many examples (see other cases of this proof and papers [1, 12, 17, 18, 19]) of tubulenes such that the resonance graph contains an isolated vertex, i. e. a path P_1 .
2. If $n = 2$, let T be a tubulene in Figure 5. Obviously, since only hexagon h_1 is a sextet, a graph in Figure 5 is a connected component of the resonance graph $R(T)$. Although there are also other perfect matchings of T , one connected component of its resonance graph is a path P_2 .
3. If $n \geq 3$, let T be a tubulene in Figure 6. Clearly, the resonance graph contains a path on n vertices $M_1M_2 \dots M_n$ and two isolated vertices M_{n+1} and M_{n+2} .

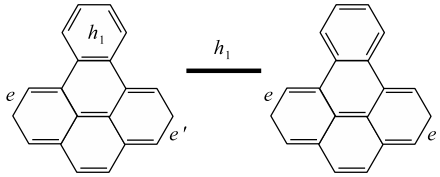


Figure 5: A connected component of the resonance graph of a tubulene in Case 2. Edges e and e' are joined together.

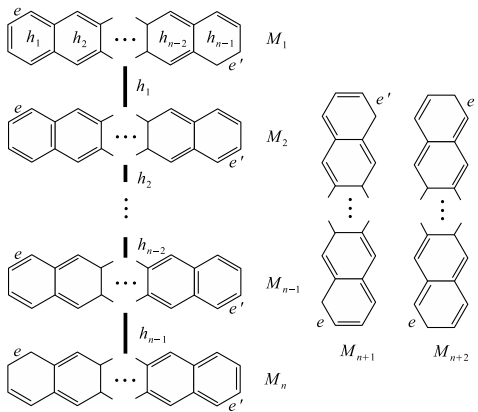


Figure 6: The resonance graph of a tubulene in Case 3. Edges e and e' are joined together.

■

It is well known fact that the resonance graph of a benzenoid system B is a path P_n , $n \geq 2$, only in the case when B is composed of $n - 1$ linearly connected hexagons. But we can find different tubulenes such that the resonance graph contains a path P_n as a connected component. See Example 3.5. To find such an example we use Lemma 3.4. A similar result has been already obtained in [13] where it was shown that every directed resonance graph of a plane bipartite graph is a Cartesian product of directed resonance graphs of its elementary components. This result could be applied in our case with some modifications but in the sake of clarity we provide a proof adapted for spherical benzenoid systems.

Lemma 3.4 *Let B be a spherical benzenoid system with a perfect matching. Let G and H be spherical benzenoid systems which are subgraphs of B such that $V(B) = V(G) \cup V(H)$ and $V(G) \cap V(H) = \emptyset$. If every edge of B with one vertex in G and another in H is a forbidden edge, then the resonance graph $R(B)$ is isomorphic to the Cartesian product of resonance graphs $R(G)$ and $R(H)$.*

Proof. We can find an isomorphism $f : R(B) \rightarrow R(G) \square R(H)$. Let $M \in V(R(B))$. Obviously, M is a perfect matching of B and since every edge between G and H is forbidden, $M = M_1 \cup M_2$ where $M_1 = M \cap E(G)$ is a perfect matching of G and $M_2 = M \cap E(H)$ is a perfect matching of H . Define $f(M) = (M_1, M_2)$ for every $M \in V(R(B))$. It is clear that $f(M) \in V(R(G) \square R(H))$. It is obvious that f is a bijection. To show that f is an isomorphism we must check that for every $M, N \in V(R(B))$ it holds: M and N are adjacent in $R(B)$ if and only if $f(M) = (M_1, M_2)$ and $f(N) = (N_1, N_2)$ are adjacent in $R(G) \square R(H)$. To do this, let M, N be two adjacent vertices in $R(B)$. Therefore, there is a hexagon h in B such that $M \oplus N = E(h)$. It is obvious that h is a hexagon in G or a hexagon in H , but not in both. If h is in G , then the vertices M_1 and N_1 are adjacent in G and $M_2 = N_2$, hence (M_1, M_2) and (N_1, N_2) are adjacent in the product. The same conclusion follows if h is in H . To see the other implication, let (M_1, M_2) and (N_1, N_2) be adjacent in the product. If M_1 is adjacent to N_1 in $R(G)$ and $M_2 = N_2$, then $M \oplus N = (M_1 \oplus N_1) \cup (M_2 \oplus N_2) = E(h) \cup \emptyset = E(h)$ for some hexagon h in G . Therefore, M and N are adjacent in $R(B)$. The same is true if $M_1 = N_1$ and M_2, N_2 are adjacent in $R(H)$. The proof is complete. ■

Example 3.5 *In Figure 7 we can see a tubulene T and three of its perfect matchings which form a connected component P_3 in the resonance graph. Obviously, using similar tubulenes one can obtain a path P_n ($n \geq 3$) as a connected component of the resonance graph. Note that although these tubulenes are all different from tubulenes in the proof of Theorem 3.3, we get a path as a connected component in the resonance graph in both cases. We also notice that edges f and f' are forbidden in tubulene T . Hence, by Lemma 3.4 the resonance graph is the Cartesian product of the resonance graphs of tubulene G (composed of three linearly connected hexagons) and benzenoid system H (with hexagons h_1 and h_2). Since $R(G)$ is a graph composed of four isolated vertices and $R(H) = P_3$ it follows that $R(T)$ has four connected components and each of them is P_3 .*

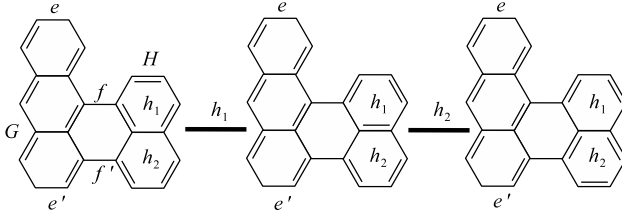


Figure 7: A connected component of the resonance graph of a tubulene. Edges e and e' are joined together.

Definition 3.6 Let T be a tubulene and \overrightarrow{OA} its chiral vector. If the graph distance between O and A is strictly more than eight, then T is called a **thick tubulene**.

In the last theorem we will prove that for thick tubulenes every connected component of the resonance graph (which is not a path) without vertices of degree one is 2-connected.

Theorem 3.7 Let T be a thick tubulene with a perfect matching. Furthermore, let H be a connected component of the resonance graph $R(T)$ such that H is not a path. If $V_1(H)$ is the set of all vertices in H that have degree one, then the graph induced on $V(H) - V_1(H)$ is 2-connected.

Proof. Let G be a subgraph of H induced on vertices in $V(H) - V_1(H)$. Since H is connected and vertices in $V_1(H)$ have degree one, it is obvious that G is connected. It is enough to prove the following: for any 2-path $M_1M_2M_3$ in G there is another path $M_1M'_2 \dots M_3$ in $H - V_1(H)$ joining M_1 and M_3 which is internally vertex disjoint with $M_1M_2M_3$. It is easy to see that if this is true, then there can be no cut vertex in G .

So let $M_1M_2M_3$ be a 2-path in G . Suppose that h_1 and h_2 are such hexagons of T that $M_2 = M_1 \oplus E(h_1)$ in $M_3 = M_2 \oplus E(h_2)$, so h_1 is an M_1 -alternating cycle and h_2 is an M_2 -alternating cycle. If h_1 and h_2 are edge disjoint, we can find another perfect matching M'_2 in G such that $M'_2 = M_1 \oplus E(h_2)$ and $M_3 = M'_2 \oplus E(h_1)$. Obviously, $M_1M'_2M_3$ is another path joining M_1 and M_3 .

If h_1 and h_2 are edge joint, then by Lemma 3.1, since the degree of M_1 in H is greater than one, there is another hexagon h_3 which is an M_1 alternating cycle and is edge disjoint with h_1 . Consider the following options:

1. If h_2 and h_3 are edge disjoint, then there is another path $M_1M'_2M'_3M'_4M_3$ joining

M_1 and M_3 , such that $M'_2 = M_1 \oplus E(h_3)$, $M'_3 = M'_2 \oplus E(h_1)$, $M'_4 = M'_3 \oplus E(h_2)$ and $M_3 = M'_4 \oplus E(h_3)$. See Figure 8.

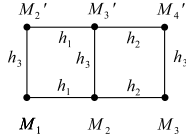


Figure 8: A part of the resonance graph of a tubulene in Case 1.

2. If h_2 and h_3 are edge joint, since the degree of M_3 in H is greater than one, by Lemma 3.1 there is another hexagon h_4 of T which is an M_3 -alternating cycle. We can easily see that h_2 and h_4 are edge disjoint.

- (a) If h_1 and h_4 are edge disjoint, then h_4 is also an M_1 -alternating cycle. Similarly as in 1. we can get a path $M_1M'_2M'_3M'_4M_3$ joining M_1 and M_3 , where $M'_2 = M_1 \oplus E(h_4)$, $M'_3 = M'_2 \oplus E(h_1)$, $M'_4 = M'_3 \oplus E(h_2)$ and $M_3 = M'_4 \oplus E(h_4)$.
- (b) If h_1 and h_4 are edge joint, we get a situation in Figure 9. Clearly, there is another path $MM'_1M'_2M'_3M'_4M'_5M_3$, where $M'_1 = M_1 \oplus E(h_3)$. $M'_2 = M'_1 \oplus E(h_1)$, $M'_3 = M'_2 \oplus E(h_4)$, $M'_4 = M'_3 \oplus E(h_3)$, $M'_5 = M'_4 \oplus E(h_2)$ and $M_3 = M'_5 \oplus E(h_4)$.

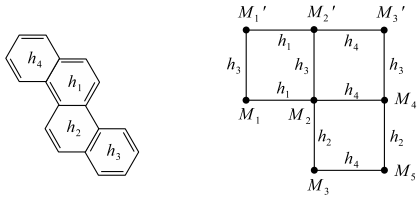


Figure 9: A perfect matching M'_1 and a part of the resonance graph in Case 2 (b).

Assumption that T is a thick tubulene is needed since otherwise a part of a tubulene in Figure 9 could be glued together and hexagons h_3 and h_4 would not be disjoint. Therefore, perfect matching M'_3 in the last case would not exist.

With this we have proved that G can not contain a cut vertex, therefore, G is 2-connected. ■

However, there also exist tubulenes that are extremely thin. For example, in [16] it was shown that a stable (2, 2)-type tubulene can be grown inside a multi-walled carbon nanotube. Note that if T is not a thick tubulene, then the subgraph of H induced on vertices $V(H) - V_1(H)$ is not necessarily 2-connected. See an example in Figure 10 (from [12]) where H is a connected component with seven perfect matchings (vertices). Edges e and e' are joined together. Obviously, H is not a path and contains a cut vertex. Therefore, the graph induced on $V(H) - V_1(H)$ is not 2-connected.

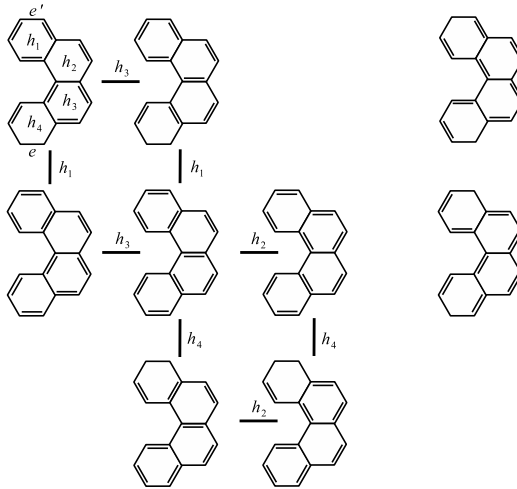


Figure 10: A tubulene such that its resonance graph contains a connected component which is not a 2-connected graph and not a path.

We will conclude the paper with an example of a tubulene T such that there exists a connected component of the resonance graph of T , different from a path, with a vertex of degree one (so $V_1(H)$ in Theorem 3.7 is not always an empty set). An example of such a tubulene can be seen in Figure 11. We can easily see that edges f and f' are forbidden edges. Hence, by Lemma 3.4, its resonance graph $R(T)$ is the Cartesian product of $R(G)$ and $R(H)$. Since $R(G)$ is composed of four isolated vertices, $R(T)$ is composed of four connected components, each isomorphic to $R(H)$. One connected component is in Figure 11.

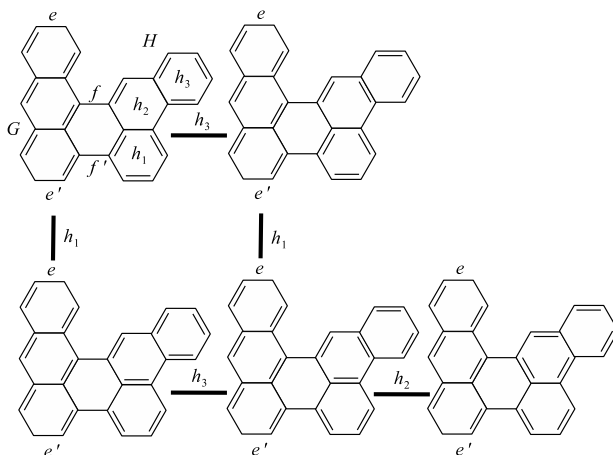


Figure 11: A tubulene (edges e and e' are joined together) and a connected component of its resonance graph which contains a vertex of degree one.

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