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ORIGINAL PAPER

On the anti-Kekulé number of leapfrog fullerenes

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Abstract The Anti-Kekulé number of a connected graph G is the smallest number of edges that have to be removed from G in such way that G remains connected but it has no Kekulé structures. In this paper it is proved that the Anti-Kekulé number of all fullerenes is either 3 or 4 and that for each leapfrog fullerene the Anti-Kekulé number can be established by observing finite number of cases not depending on the size of the fullerene.

Keywords Anti-Kekulé number · Fullerene · Leapfrog fullerene

1 Introduction

Graph theory models have been extensively used as predictors of the properties of chemical compounds (see [1,2] and references within). The concept of perfect matchings [3] corresponds to the notion of Kekulé structure in chemistry and plays a very important role in analyses of benzenoid systems, fullerenes and other carbon cages [4,5]. For example, it is well known that carbon compounds without Kekulé structures are unstable.

Fullerenes are closed carbon-cages that contain only pentagonal and hexagonal rings. For the discovery of the first fullerene C_{60} [6,7] R. F. Curl, H. Kroto and

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R. E. Smalley received the Nobel Prize. The study of Kekulé structures of chemical compounds is very important, because they have many "hidden treasures" [5] that may explain their physical and chemical properties. Kekulé structures of C_{60} have been extensively studied by M. Ranić, H. Kroto, D. Vukičević and others [8–11].

It is found that the anti-Kekulé number [12] of C_{60} is equal to 4 [13]. The aim of this paper is to extend this result to the class of leapfrog fullerenes. Note that C_{60} is the smallest leapfrog fullerenes [14]. All leapfrog fullering obey the IP (isolated pentagon rules), that is they don't have adjacent pentagons [14]. It is claimed that fullerenes that obey IP are the most stable and the most important fullerenes [14], hence their study is of great interest.

2 Basic definitions and preliminaries

Let G be a connected graph with at least one perfect matching (Kekulé structure). Denote by $E(G)$ the set of its edges and by $V(G)$ the set of its vertices. Let $S \subseteq E(G)$. Denote by $G - S$ the graph obtained from G by eliminating edges in S. If $G - S$ is connected and has no perfect matching, then we say that S is an anti-Kekulé set. The cardinality of the smallest anti-Kekulé set is called the anti-Kekulé number of G and is denoted by $ak(G)$.

Also, in graph theory a fullerene is defined as any 3-connected 3-regular, planar graph with all faces of size 5 or 6 (including the external face). From Euler's polyhedron formula it follows that there are exactly 12 pentagons in a fullerene.

To define the leapfrog transformation of a fullerene we have to introduce stellation and dualization [15]. Stellation, St, of a face is achieved by adding a new vertex in its center followed by connecting it with each boundary vertex. It is also called a capping operation or triangulation. When all the faces of a graph are thus operated on, it is referred to as an omnicapping operation and the resulting graph is denoted by $St(G)$. Dualization, Du, of a graph is built as follows: locate a point in the center of each face. Join two such points if their corresponding faces have a common edge. The new edge is called the edge dual, $Du(e)$ and the transformed map, the (Poincaré) dual $Du(G)$. The vertices of $Du(G)$ represent the faces of G and vice-versa. Dual of the dual recovers the original graph: $Du(Du(G)) = G$. Leapfrog, Le, is a composite operation that can be written as: $Le(G) = Du(St(G))$. Vertices that are added in the stellation of a graph, and faces that correspond to those vertices in the dual of a stellation will be called *caps*, other faces will be referred to as *non-caps*.

Also, if a graph G is d-regular then the following theorem holds [15]:

Theorem 1 *The number of vertices in the leapfrog transform $Le(G)$ of G is d times larger than in the original graph G.*

Since a fullerene G is a 3-regular graph, the number of vertices in $Le(G)$ is 3 times larger than in G. Note that $Le(G)$ is a fullerene too.

3 Main results

In this paper we will investigate the anti-Kekulé number of an arbitrary leapfrog fullerene. First we will show that the anti-Kekulé number of an arbitrary leapfrog fullerene is at most 4. To show that, let G be an arbitrary leapfrog fullerene and consider one pentagon in G. Let us label the vertices of that pentagon with numbers $1, 2, 3, 4, 5$. Each of these five vertices has two neighbors on the pentagon. Since G is 3-regular, for each of these 5 vertices there is exactly one vertex adjacent to it which is not on the pentagon. Let us denote that remaining neighbor of a vertex i with v_i for $i = 1, \ldots, 5$. Now, let us choose one vertex on the pentagon, say vertex 1, and let the vertices 2 and 5 be its neighbors on the pentagon. We define the set $S = \{e_1, e_2, e_3, e_4\}$ where e_1 and e_2 are two edges incident to vertex 5 and not to vertex 1, and e_3 and e_4 are two edges incident to vertex 2 and not to vertex 1. In the graph $G - S$ vertices 2 and 5 can both be matched only with vertex 1. Therefore $G - S$ has no perfect matching (Kekulé structure). This all is illustrated in Fig. 1.

Also, we have to prove that $G - S$ remains connected. To show that, first denote the non-cap hexagon incident to the edge $i - j$ by C_{ij}. Note that by deleting the edge $2 - v_2$ the graph remains connected since it contains a path from vertex 2 to v_2 consisting of the remainder of the hexagon C_{12}. By further deleting the edge $2 - 3$ the graph still remains connected since it contains a path from 2 to 3 consisting of the remainders of hexagons C_{12} and C_{23}. The proof that G remains connected after further deletion of edges $5 - v_5$ and $4 - 5$ is analogous. This is illustrated in Fig. 2.

So, the set S of cardinality 4 is an anti-Kekulé set, hence we can conclude $ak(G) \leq 4$.

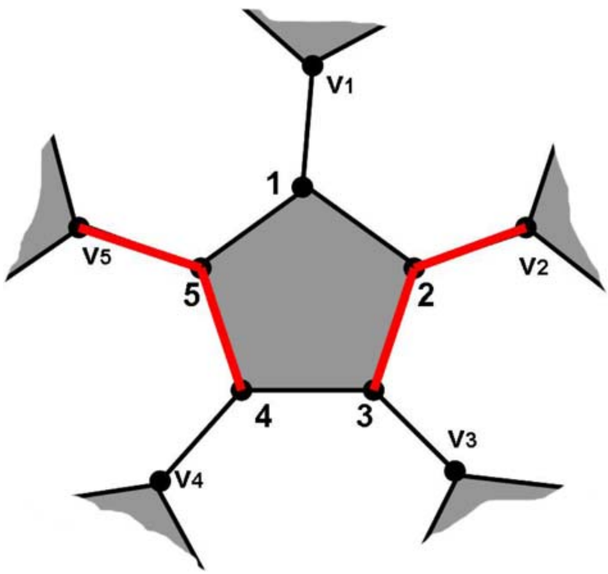

Fig. 1 The Anti-Kekulé set of cardinality four for an arbitrary fullerene

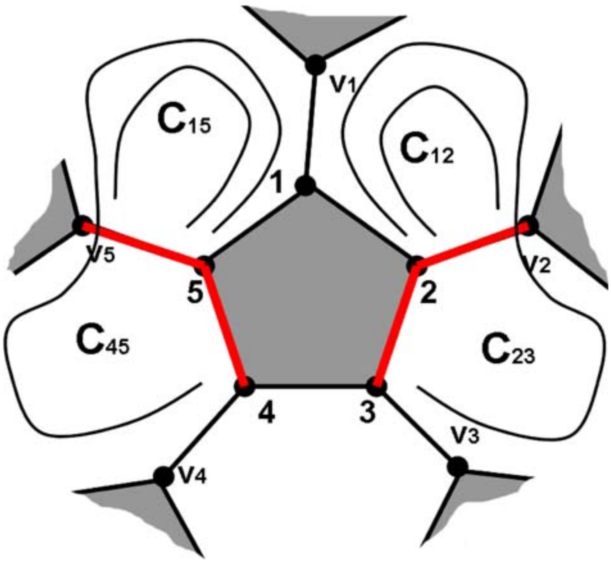

Fig. 2 Path that connect vertices incident to deleted edges

We are now ready to prove the main theorem of this paper. First, note that all non-caps in the leapfrog fullerene G are hexagons, while caps can be pentagons or hexagons where the number of pentagon caps is exactly 12.

A graph is *cyclically k-edge-connected* if at least k edges need to be removed in order to disconnect the graph into two components each containing a cycle. It was proved by Došlić ([16], Theorem 2) that the cyclic edge-connectivity of a fullerene is 5. Obviously, fullerene has no cycles of length 3 or 4. Let us prove our main theorem:

Theorem 2 *Let* $G = Le(\Gamma)$ *be an arbitrary leapfrog fullerene. If* $ak(G) = 3$ *then the smallest anti-Kekulé set is* $S = \{e_1, e_2, e_3\}$ *where*

(i) e_3 *is incident to two non-cap hexagons which are neighboring exactly two pentagon caps.*
(ii) e_1 *is incident to one of the two non-cap hexagons and one of the two pentagon caps, and*
(ii) e_2 *is incident to other of the two non-cap hexagons and other of the two pentagon caps.*

All the possibilities for S are illustrated in Fig. 3.

Proof For convenience we introduce the following terminology. An edge incident to a cap will be called a *cap edge*, and a *non-cap edge* otherwise.

Now, let G be an arbitrary leapfrog fullerene with $ak(G) = 3$ and S the smallest anti-Kekulé set. We will distinguish four different cases.

Case 1 All three edges from S are cap edges.

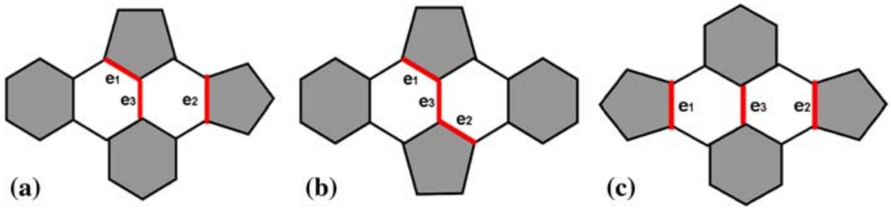

Fig. 3 All the possibilities for set S from Theorem 2

Noting that every vertex in a leapfrog fullerene G is incident to exactly one non-cap edge, we can conclude that the set of all non-cap edges is a perfect matching in G. Therefore, this case is impossible.

Case 2 Exactly two of the edges in S are cap edges.

Let us denote those two edges by e_1 and e_2. The remaining edge from S, call it e_3, is a non-cap edge. Furthermore, let us denote with H_1 and H_2 the two non-cap hexagons to which e_3 is incident. We first claim that e_1 and e_2 have to be adjacent to H_1 or H_2 too. To prove that suppose on the contrary, that at least one of the edges e_1 and e_2 is not incident to any of the hexagons H_1 and H_2. We will construct a perfect matching in $G - S$ as follows. Let all vertices in $G - S$, except for vertices on H_1 and H_2, be matched by non-cap edges. Since at most one of the cap edges on H_1 and H_2 is in S, it follows that for at least one of the hexagons H_1 and H_2, all three cap edges incident to it in G are included in $G - S$ too. Without loss of generality we can assume that hexagon be H_1. Then the vertices from H_1 can be matched by cap edges, and the remaining four vertices from H_2 can be matched by non-cap edges. Therefore we have a perfect matching in $G - S$, which is a contradiction. This is illustrated in Fig. 4.

Now, consider a patch on a fullerene consisting of two non-cap hexagons H_1 and H_2 to which that one non-cap edge e_3 from S is incident to, four caps adjacent to those two hexagons and all non-cap hexagons adjacent to those four caps. It can be checked that $G - S$ has a perfect matching in all cases except when exactly two out of four caps adjacent to H_1 and H_2 are pentagons, say P_1 and P_2, and $e_1 \in S$ is adjacent to H_1 and P_1 while $e_2 \in S$ is adjacent to H_2 and P_2. These exceptions are precisely the ones shown in Fig. 3.

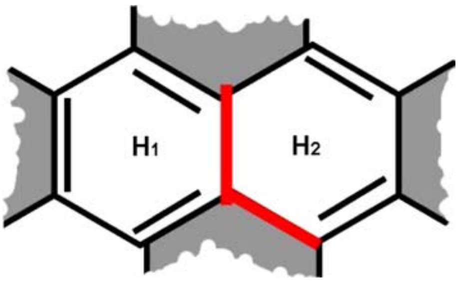

Fig. 4 An example of matching vertices on H_1 and H_2. Cap faces are shown in grey. Edges from S are red

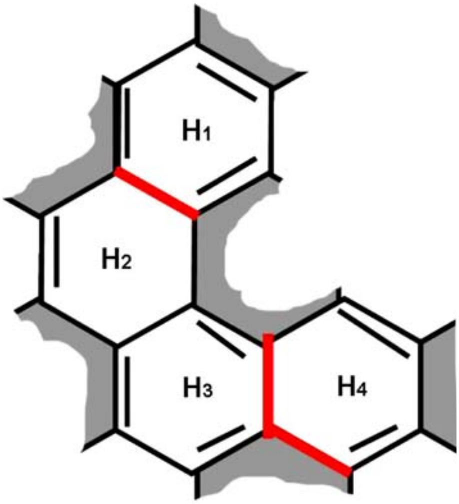

Fig. 5 A matching of vertices on hexagons H_1, H_2, H_3 and H_4

Case 3 Exactly one of the edges in S is a cap edge, denote it by e_1. The remaining two non-cap edges from S are e_2 and e_3.

First we claim that e_2 and e_3 belong to the same non-cap hexagon. Suppose on the contrary, that H_1 and H_2 are the two non-cap hexagons containing e_2, and H_3 and H_4 are the two non-cap hexagons containing e_3, in total four different hexagons. Now we construct a perfect matching as follows. All vertices from $G - S$ except for vertices from H_1, H_2, H_3 and H_4 are matched using non-cap edges. Since only one cap edge is in S, it follows that for at least three of the hexagons H_1,H_2, H_3 and H_4, all three cap edges incident to it are included in $G - S$. Without loss of generality we can suppose that these hexagons are H_1, H_2 and H_3. It follows then vertices on H_3 can be matched by cap edges, and the remaining vertices on H_4 by non-cap edges. Since non-cap hexagons correspond to vertices in Γ and Γ has no cycles of length 3 or 4, it follows that at least one of the hexagons H_1 and H_2 is not adjacent to either of the hexagons H_3 and H_4. Without loss of generality we can assume that this hexagon is H_1. It follows that vertices on H_1 are matched by cap edges, and the remaining vertices on H_2 are matched by non-cap edges. This is illustrated in Fig. 5.

In conclusion e_2 and e_3 have to be contained on the same non-cap hexagon H for otherwise $G - S$ has a perfect matching. Further, we claim that the cap edge e_1 from S also belongs to H. Namely note that if that was not the case vertices of $G - S$ not on H could be matched by non-cap edges and vertices on H could be matched by cap edges. This would gives us a perfect matching on $G - S$, a contradiction. This is illustrated in Fig. 6.

Let us now consider a patch on a fullerene which consists of a non-cap hexagon H to which all edges from S are incident, three caps adjacent to H, and all non-cap hexagons adjacent to those three caps. It is easily seen that all vertices in $G - S$ can be matched by non-cap edges. Also, it can be verified (by computer) that vertices on this patch can be perfectly matched in all possible cases. That is, irrespective of any pentagon and hexagon making up this patch.

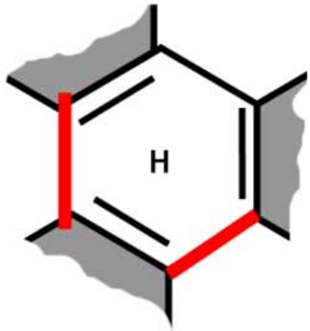

Fig. 6 An example of matching vertices on hexagon H

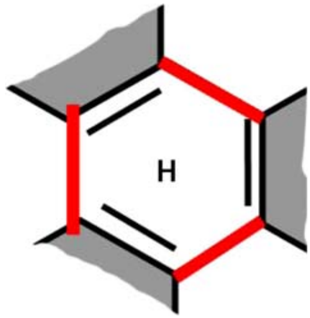

Fig. 7 An example of matching vertices of hexagon H

Case 4 None of the edges in S is a cap edge.

If all three edges from S belong to the same hexagon H then the vertices on H can be matched in $G - S$ by cap edges on H, whereas other vertices can be matched by non-cap edges. These would give us a perfect matching in $G - S$, a contradiction. This is illustrated in Fig. 7.

Now suppose that two of the edges from S belong to the same hexagon H. The remaining edge belongs to two hexagons, call them H_1 and H_2, both different form H. Since Γ does not cycles of length 3, then it follows that at least one of H_1 and H_2 is not adjacent to H. Say this hexagon is H_1. Then all vertices in $G - S$ can be matched by non-cap edges except vertices on H and H_1. These can be matched by cap edges on H and H_1. Therefore we would have a perfect matching in $G - S$, a contradiction. This is illustrated in Fig. 8.

Now suppose that the three edges from S belong to different hexagon: H_1, H_2 and H_3. Also, they can be chosen in such a way that neither two of them are adjacent. To show this, note that each of the edges from S is adjacent to two non-cap hexagons, that is, e_1 is incident to H_1 and H_1', and e_2 is incident to H_2 and H_2', and e_3 is incident to H_3 and H_3'. Since Γ does not contain cycles of length 3 and 4, it follows that at most one of the hexagons H_1 and H_1' is adjacent to at most one of hexagons H_2 and H_2'. Without loss of generality we can assume that H_1' is adjacent to H_2'. Then choose the hexagon H_1 and H_2', respectively, for edge e_1 and e_2. This is illustrated in Fig. 9.

If one of the hexagons H_3 and H_3' is not incident to either of the two hexagons H_1 and H_2', then we choose that hexagon for edge e_3 and so neither of the three chosen

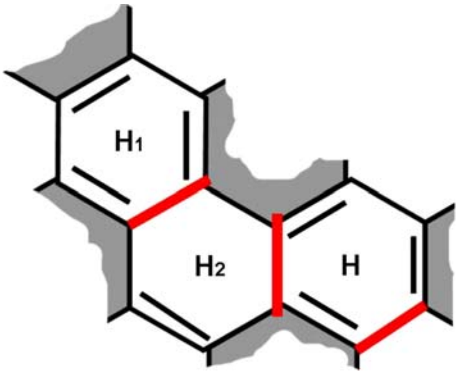

Fig. 8 An example of matching vertices of hexagons H, H_1 and H_2

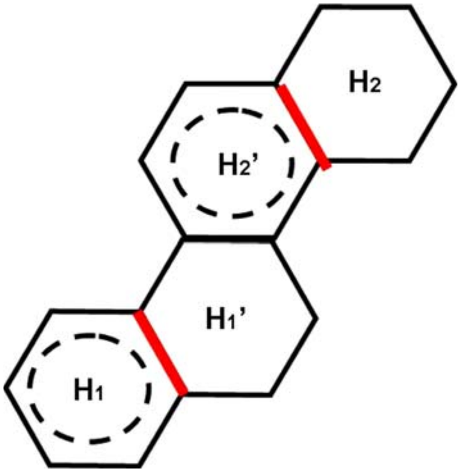

Fig. 9 Choosing hexagons H_1 and H_2 so that they are not adjacent

hexagons are adjacent. Otherwise, if say H_3 is adjacent to H_2' and H_3' is adjacent to H_1, then the fact that Γ does not contain cycles of length 3 and 4 implies that H_2 is not adjacent to any of the hexagons H_1, H_1', H_3 and H_3'. Then we can choose H_1 for e_1, H_2 for e_2 and H_3 for e_3. This is illustrated in Fig. 10.

We have shown that H_1, H_2 and H_3 can be chosen in such a way that no two of them are adjacent. It follows that all vertices in $G - S$ can be perfectly matched by non-cap edges except for vertices on H_1, H_2 and H_3. But these vertices can be perfectly matched by cap edges incident to those hexagons. We again have a perfect matching in $G - S$, a contradiction. This is illustrated in Fig. 11. This proves Theorem 2. □

Note that C_{60}, the leapfrog-fullerene of the dodecahedron, does not contain any of the three local structures shown in Fig. 3 and therefore Theorem 2 implies that $ak(C_{60}) = 4$ which is consistent with the result in [13].

Now, if we want to calculate the anti-Kekulé number of a leapfrog fullerene, from Theorem 2 it follows that we have to check at most 90 combinations of three edges. Namely, set S must contain 3 edges: e_1, e_2 and e_3, where e_1 and e_2 are cap edges and e_3 is non-cap edge. Let us first fix cap edge e_1. The cap e_1 belongs to must be

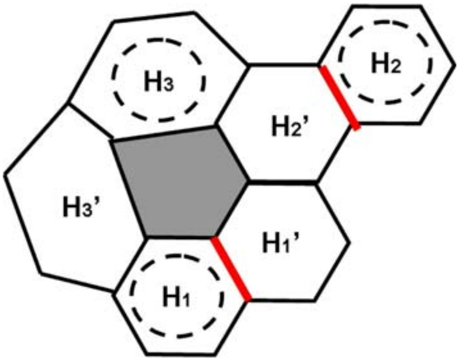

Fig. 10 Choosing hexagons H_1, H_2 and H_3 so that they are not adjacent

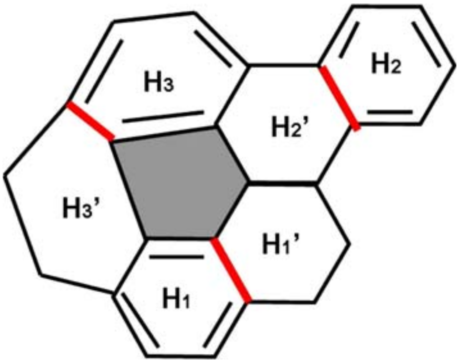

Fig. 11 An example of matching vertices of hexagons H_1, H_2 and H_3

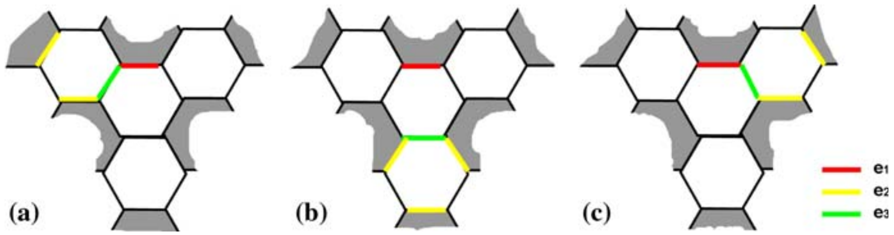

Fig. 12 Combinations of edges that must be checked in order to calculate $ak\,(G)$

pentagon, so this can be done in 60 ways since there are exactly 12 pentagon caps, each of which has 5 cap edges. Now note that the non-cap edge $e_3 \in S$ must be chosen among one of the three non-cap edges on a non-cap hexagon to which e_1 belongs to. Relative to these three choices of e_3, the remaining cap edge $e_2 \in S$ can be in at most 7 positions. This is illustrated in Fig. 12.

Note that Fig. 12a represents two possible combinations of edges, Fig. 12b represents three possible combinations of edges and Fig. 12c represents two possible combinations of edges. In each case edges e_1 and e_3 are fixed and two (or three in case b) combinations are obtained by choosing one of the two (or three in case b) marked edges for e_2. Therefore, there are 7 combinations in all. Furthermore, note that not all 7 combinations satisfy conditions of Theorem 2 at the same time. How many of

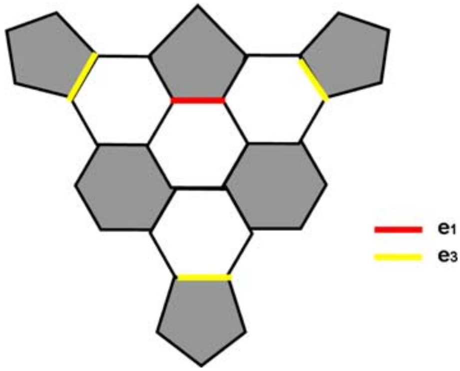

Fig. 13 The maximum possible number of admissible combinations to be checked

them do satisfy the conditions of Theorem 2, depends on the sizes of the neighboring caps. A somewhat tedious analysis shows that the maximum number of admissible combinations is 3 and is attained with respect to combination of caps shown in Fig. 13.

Therefore, e_1 can be chosen in 60 different ways, and for chosen e_1 there are at most 3 different possibilities for S. Also, note that in this way each admissible combination of edges is counted twice. Namely, since e_1 and e_2 are both cap edges that belong to a pentagon cap, the same combination is counted second time with e_2 in the place of e_1 and e_1 in the place of e_2. So, we can conclude that there are at most $60 \cdot 3/2 = 90$ possible combinations for S.

4 Conclusions

In this paper, it is established that the anti-Kekulé number of a leapfrog fullerene is either 3 or 4. In particular, it is shown that only leapfrog fullerenes with the anti-Kekulé number equal to 3 are those which contain at least two pentagons at distance 2 (that is, with precisely one hexagon between these two pentagons). In particular, the anti-Kekulé number of the leapfrog fullerene of a fullerene obeying IPR is equal to 4. Consequently, the anti-Kekulé number of the leapfrog fullerene of any leapfrog fullerene is equal to 4.

Also, it is shown that the anti-Kekulé number can be computed by an analysis of at most 90 cases. This result dramatically reduces the time needed for finding the anti-Kekulé number of fullerenes in the generale case. Let us illustrate this by a simple example. Consider the leapfrog fullerene $Le\ (C_{60})$, where C_{60} is any fullerene with 60 vertices (not necessarily Buckminsterfullerene). $Le\ (C_{60})$ has 180 vertices and hence 270 edges. Without this theorem, one would have to consider $\binom{270}{3} = 3{,}244{,}140$ cases, but here it is shown that it is sufficient to observe only 90 cases. Moreover if C_{60} is Buckminsterfullerene (which obeys the IP), the anti-Kekulé number of $Le(C_{60})$ is equal to 4and no cases need to be analyzed.

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