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On the anti-forcing number of benzenoids

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The anti-forcing number is introduced as the smallest number of edges that have to be removed that any benzenoid remains with a single Kekulé structure. Similarly, the anti- Kekulé number is discussed as the smallest number of edges that have to be removed that any benzenoid remains connected but without any Kekulé structure. These concepts have been exemplified on damaged benzenoid parallelograms.

KEY WORDS: anti-forcing number, benzenoids, forcing number, damaged benzenoid paralleograms

1. Introduction

The *forcing number* of benzenoids has been introduced in this journal about 15 years ago by Harary et al. [1]. The roots of this concept can be found in an earlier paper by Randić and Klein [2]. There, the forcing number has been called the *innate degree of freedom* of a Kekulé structure, although the term the forcing number was also used. The forcing number is equal to the *smallest* number of double bonds that completely determines the Kekulé structure of a given benzenoid. After this initial report, several papers appeared reporting the forcing number of hexagonal systems and square grids [e.g., 3,4].

Recently, the *total* (or *global*) forcing number is defined in the following way [5]: let $G = (V(G), E(G))$ be a graph G with a perfect matching (or Kekulé structure). Denote by $K(G)$ the set of all Kekulé structures in G and consider functions $f_S : K(G) \to \{0, 1\}^S$ defined by:

$$[f_S(\kappa)]_i = \begin{cases} 1, & e_i \in \kappa, \\ 0, & e_i \notin \kappa. \end{cases} \tag{1}$$

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If f_S is an injection, then S is *global* forcing set. A global forcing set of the smallest cardinality is called a minimal global forcing set, and its cardinality is the global forcing number of G.

In the present report, we introduce a quantity that is opposite to the forcing number that we call the *anti-forcing number*.

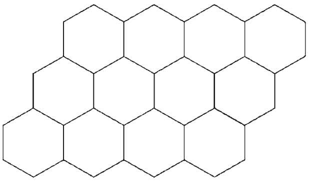
2. Definitions

Let $G = (V(G), E(G))$ be a graph G with a perfect matching. Anti-forcing set of G is the set S such that G-S has a unique Kekulé structure. Anti-forcing set of the smallest cardinality is called the minimal anti-forcing set, and its cardinality is the anti-forcing number of G and we denote it by $af(G)$.

Anti-Kekulé set of G is the set S such that G-S is a connected graph and it has no Kekulé structures. Anti-Kekulé set of the smallest cardinality is called a minimal anti-Kekulé set, and its cardinality is the anti-Kekulé number of G and we denote it by $ak(G)$.

In our recent paper [6], the *damaged* benzenoids are analyzed. Here, we consider the anti-forcing number as the smallest number of edges that have to be removed (damaged) in order that G remains with a single Kekulé structure. We also consider the anti-Kekulé number of G as the smallest number of edges that have to be removed (damaged) in order that G remains connected, but without any Kekulé structures.

As in our earlier papers [6,7], we consider parallelogram-like shaped benzenoids, called *benzenoid parallelograms* [8–10], $B_{m,n}$ consisting of $m \times n$ hexagons, arranged in m rows, each row consisting of n hexagons. We ilustrate this by presenting benzenoid $B_{3,4}$:



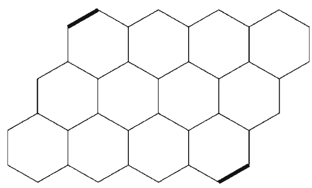
$B_{3,4}$

3. Theorems

Let us prove the following theorem:

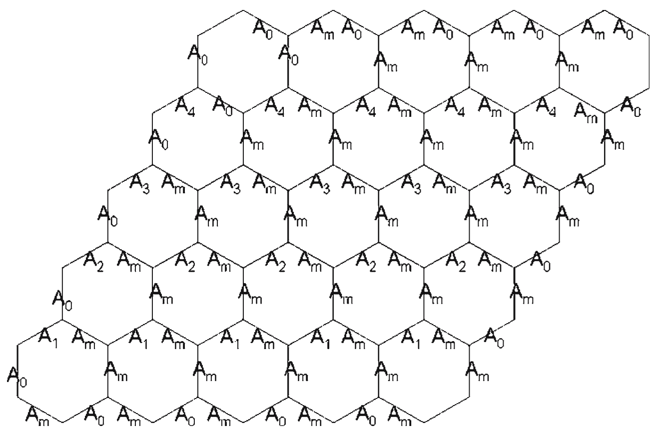
Theorem 1. $af\left(B_{m,n}\right) = 1,\ m, n \geqslant 3.$

Note there are only two minimal-anti-forcing sets, each consisting of one bold edge in the following figure:

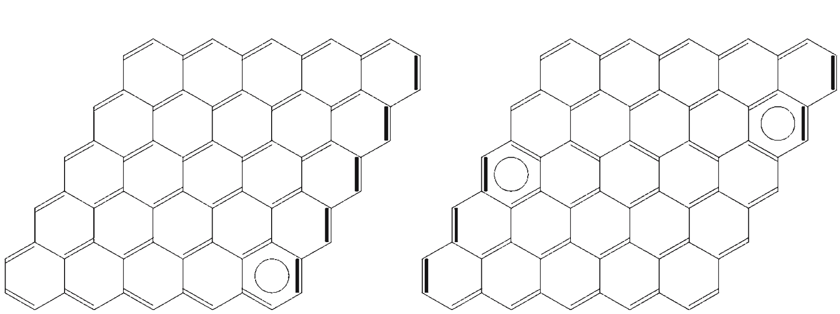


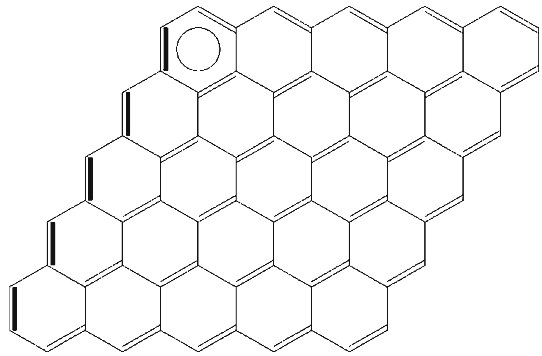
Proof. Denote the upper bold edge by e_1 and lower bold edge by e_2. Obviously, $af\left(B_{m,n}\right) \geqslant 1$. In the paper by Lukovits et al. [6], it is shown that $B_{m,n} - e_2$ has a unique Kekulé structure and by symmetry it follows that $B_{m,n} - e_1$ also has a unique Kekulé structure. It is sufficient to show that $B_{m,n} - e$ has at least two Kekulé structures for each $e \in E\left(B_{m,n}\right) - \{e_1, e_2\}$.

Let us partition all edges in $E\left(B_{m,n}\right) - \{e_1, e_2\}$ to classes $A_0, A_1, A_2, \ldots, A_m$ as illustrated below in the case of $B_{5,5}$:



Further, denote by K_x the Kekulé structure that contains x lower left-most vertical double bonds and m–x upper right-most vertical double bonds. The examples for K_0, K_3 and K_5 in $B_{5,5}$ are presented below:

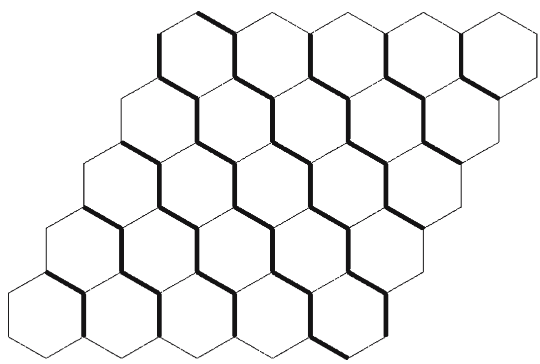




Denote by K_0' the Kekulé structure that is obtained from K_0 by rotating three double bonds in the hexagon denoted by circle. Note that K_0 and K_0' are two Kekulé structures on $B_{m,n}$–e for each $e \in A_0$. Denote by K_m' the Kekulé structure that is obtained from K_m by rotating three double bonds in the hexagon denoted by circle. Note that K_m and K_m' are two Kekulé structures on $B_{m,n}$–e for each $e \in A_m$.

Let $1 < i < m$. Denote by K_i' the Kekulé structure that is obtained from K_i by rotating three double bonds in the left hexagon denoted by circle and denote by K_i'' the Kekulé structure that is obtained from K_i by rotating three double bonds in the right hexagon denoted by circle. Note that for each $e \in A_i$ at least two of K_i, K_i' and K_i'' (Kekulé structures of $B_{m,n}$) are Kekulé structures of $B_{m,n} - e$. Hence, for each $e \in E\left(B_{m,n}\right) - \{e_1, e_2\}$, there are at least two Kekulé structures of $B_{m,n} - e$. □

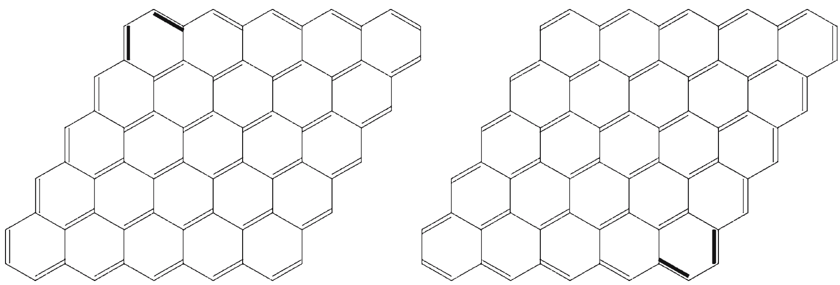
Let us divide edges of $B_{m,n}$ in two classes E_1 and E_2, where edges in E_1 are drawn with normal lines and edges of E_2 with bold lines as shown below:



Theorem 2. $ak\left(B_{m,n}\right) = 2$, $m, n \geqslant 3$. Moreover, for every edge $e \in E_1$, there is minimal anti-Kekulé set that contains e. There is no minimal anti-Kekulé set that contains any edge in E_2.

Proof. In the proof of Theorem 1, it is shown that for each $e \in E\left(B_{m,n}\right)$, $B_{m,n}$–e has at least one Kekulé structure. Hence, $ak\left(B_{m,n}\right) \geqslant 2$.

Now, let us prove that for every edge $e \in E_1$, there is the (minimal) anti-Kekulé set with two elements that contains e (this would also imply that $ak\left(B_{m,n}\right) \leqslant 2$). Denote e_1 and e_2 as in the proof of theorem 1. It is pointed out there that $B_{m,n}$–e_1 and $B_{m,n}$–e_2 have exactly one Kekulé structure. These Kekulé structures are given below:



Denote by E_1' the set of non-bold double bonds in the left figure and denote by E_1" the set of non-bold double bonds in the right figure. Note that $E = \{e_1, e_2\} \cup E_1' \cup E_1''$. Distinguish 2 cases:

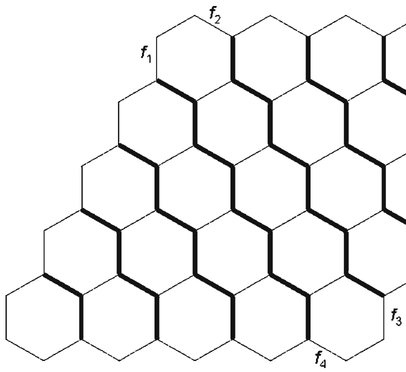
Case 1. $e = e_1$ or $e = e_2$.

Since both equalities are analogous, we may assume that $e \in e_1$. Let $e' \in E_1'$ be any edge. Since, $B_{m,n}$–e_1 has the only *one* Kekulé structure and e' is double bond in this structure, it follows that $B_{m,n}$–$e_1 - e'$ has *no* Kekulé structures. One can easily see that $B_{m,n} - e_1$–e' is connected. Hence, $\left\{e_1, e'\right\}$ is the minimal anti-Kekulé set.

Case 2. $e \in E_1^{'}$ or $e \in E_1''$.

Since both equalities are analogous, we may assume that $e \in E_1'$. Since there is only *one* Kekulé structure on $B_{m,n}$–e_1, then there are *no* Kekulé structures on $B_{m,n}$–$e_1 - e$. One can easily see that $B_{m,n}$–e_1 –e' is connected. Therefore $\{e, e_1\}$ is minimal anti-Kekulé set on $B_{m,n}$.

It remains to prove that each $e \in E_2$ is *not* contained in any minimal anti-Kekulé set. Divide E_2 in three sets $E_2 = E_2' \cup E_2'' \cup \{f_1, f_2, f_3, f_4\}$ where edges of E_2' are drawn with vertical bold lines and edges of E_2'' with non-vertical bold lines as in $B_{5,5}$ shown below:

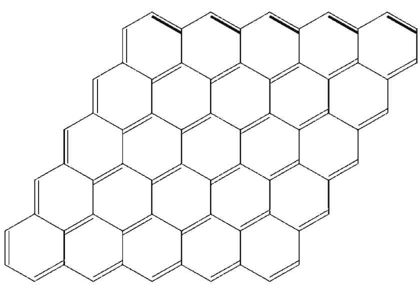


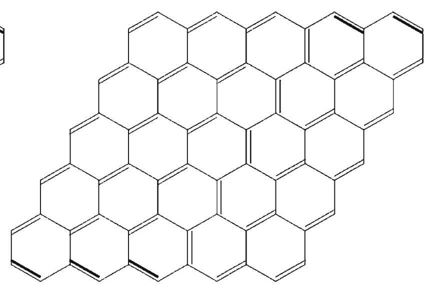
Case 1. $e \in E_2'$.

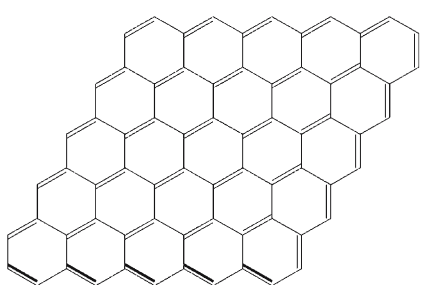
Suppose that $\{e, e'\}$ is the minimal anti-Kekulé set for some $e' \in E\left(B_{m,n}\right)$. Denote $K_0, K_1, \ldots, K_m$ as in the proof of the last theorem. Denote by $s\left(K_i\right)$ the set of single edges of Kekulé structure K_i. Note that $e \in s\left(K_i\right)$ for each $i = 0, \ldots, m$. Also note that $E\left(B_{m,n}\right) = \bigcup_{i=0}^{m} s\left(K_i\right)$. Hence, there is K_i such that $\{e, e'\} \in s\left(K_i\right)$, but then K_i is the Kekulé structure on $B_{m,n} \backslash \{e, e'\}$. This is contradiction.

Case 2. $e \in E_2''$.

Suppose that $\{e, e'\}$ is the minimal anti-Kekulé set for some $e \in E\left(B_{m,n}\right)$. Denote by H_x the Kekulé structure that contains x left lower-most downward double bonds and m–x right upper-most vertical double bonds. The examples for H_0, H_3, and H_5 in $B_{5,5}$ are presented below:



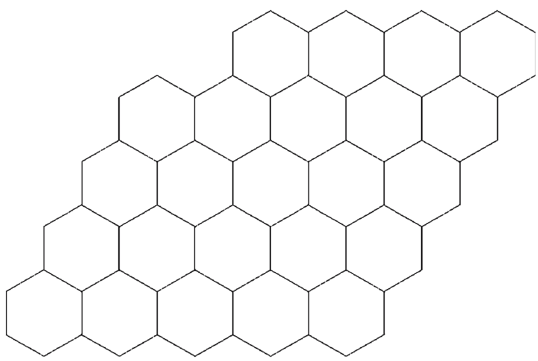




Denote by $s(H_i)$ the set of single edges of the Kekulé structure K_i. Note that $e \in s(H_i)$ for each $i = 0, \ldots, m$. Also note that $E\left(B_{m,n}\right) = \bigcup_{i=0}^{m} s(H_i)$. Hence, there is H_i such that $\left\{e, e'\right\} \in s(H_i)$, but then H_i is the Kekulé structure on $B_{m,n} \setminus \left\{e, e'\right\}$. This is contradiction.

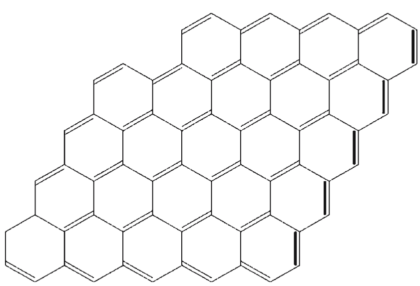
Case 3. $e \in \{f_1, f_2, f_3, f_4\}$.

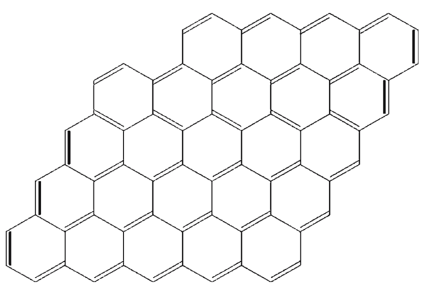
Because of the symmetry, we may assume that $e \in \{f_1, f_2\}$. Suppose that $\left\{e, e'\right\}$ is the minimal anti-Kekulé set. Note that $e' \neq e_1$, because $B_{m,n}$–e–e_1 is disconnected. It follows that $B_{m,n}$ –e–e' has a Kekulé structure if and only if $B'_{m,n}$–e' has a Kekulé structure when $B'_{m,n}$ is obtained form $B_{m,n}$ by deletion of the left-upper hexagon. Damaged $B_{5,5}$ denoted by$B'_{5,5}$ is shown below:

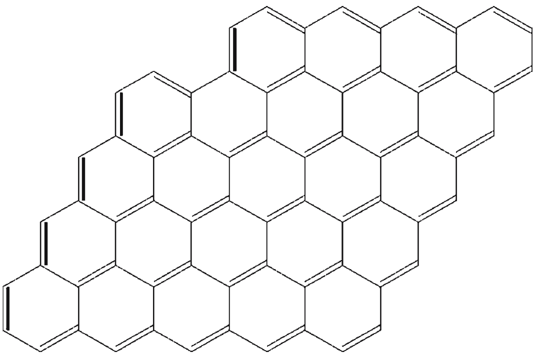


$B'_{5,5}$

Define $K'_0, K'_1, \ldots, K'_m$ analogously as $K_0, K_1, \ldots, K_m$. Examples for K'_0, K'_3, and K'_5 in $B_{5,5}$ are given below:







Define $s\left(K_i'\right)$ analogously as before and note that $E\left(B_{m,n}'\right) = \bigcup_{i=0}^{m} s\left(K_i'\right)$. Hence, there is K_i' that does not contain e'. This is contradiction. □

4. Conclusion

The concept of forcing number of benzenoids is known for sometime. It is defined as the smallest number of double bonds that completely determines the Kekulé structure of any benzenoid. Here, we introduced the anti-forcing number as the smallest number of edges that have to be removed from a benzenoid to remain with a single Kekulé structure. Additionally, we introduced the anti-Kekulé number as the smallest number of edges that have to be removed from a benzenoid so that it remains connected, but without any Kekulé structure. These concepts have been illustrated on damaged benzenoid parallelograms, that is parallelogram-like shaped benzenoids with selected edges removed (damaged).

Acknowledgments

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References

[1] F. Harary, D.J. Klein and T.P. Živković, Graphical properties of polyhexes: perfect matching vector and forcing, J. Math. Chem. 6 (1991) 295–306.

[2] M. Randić and D.J. Klein, Kekulé valence structures revisited. Innate degrees of freedom of pi-electron couplings, in: *Mathematics and Computational Concepts in Chemistry*, ed. N. Trinajstić (Horwood/Wiley, New York, 1986, pp. 274–282.

[3] F. Zhang and X. Li, Hexagonal systems with forcing edges, Discrete Math. 140 (1995) 253–263.

[4] L. Plachter and P. Kim, Forcing number on square grid, Discrete Math. 190 (1998) 287–294.

[5] D. Vukičević and J. Sedlar, Total forcing number of the triangular grid, Math. Commun. 9 (2004) 169–179.

[6] I. Lukovits, A. Milićević, N. Trinajstić and D. Vukičević, Kekulé-structure counts in damaged benzenoid parallelograms, Internet Electronic J. Mol. Des.

[7] D. Vukičević, I. Lukovits and N. Trinajstić, Counting Kekulé structures of benzenoid parallelograms containing one additional benzene ring, Croat Chem. Acta.
[8] S.J. Cyvin and I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons* (Springer, Berlin, 1988).
[9] N. Trinajstić, *Chemical Graph Theory*, 2nd ed. eition (CRC, Boca Raton, FL, 1992).
[10] T. Došlić, Perfect matchings in lattice animals and lattice paths with constraints, Croat. Chem. Acta 78 (2005) 251–259.