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Resonant Sets of Benzenoid Graphs and Hypercubes of Their Resonance Graphs

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Abstract

It is shown that if G is an elementary benzenoid graph without nice coronenes then there exists a bijective mapping from the set of subgraphs of the resonance graph $R(G)$, that are maximal hypercubes into the set of maximal resonant sets of G. In addition to this a connection between alternating sets of G and a subgraphs of $R(G)$ that are maximal hypercubes is presented.

1 Introduction

Benzenoid graphs are investigated in chemical graph theory [1, 2] since they represent the chemical compounds known as benzenoid hydrocarbons. A necessary condition for a benzenoid hydrocarbon to be (chemically) stable is that it possesses Kekulé structures, which describe the distribution of so called π-electrons.

The resonance graph or a Z-transformation graph [3] of a benzenoid graph models interactions among its Kekulé structures. The vertices of the resonance graph are the Kekulé structures; two vertices are adjacent if the corresponding Kekulé structures interact, that is if one Kekulé structure is obtained from the other by rotating three double bonds in a hexagon. This concept of resonance graphs was first put forward by Gründler

[4] and was then re-invented by El-Basil [5, 6] and, independently, by Randić [2]. In addition to this, without any reference to chemistry, where instead of searching for Kekulé structures we are interested in perfect matchings of a more general family of graphs, i.e. plane bipartite graphs, Zhang, Guo and Chen introduced resonance graphs under the name Z-transformation graphs and established their basic mathematical properties [3, 7, 8]. For some recent developments see the survey paper [9]. One of the most important properties established by Lam et al. [10] is that the resonance graphs are median graphs.

The main motivation for this paper is the result from [11] saying, that there exists a one-to-one mapping from the set of subgraphs of $R(G)$ isomorphic to the $Cl(G)$-dimensional hypercube into the family of maximum cardinality resonant sets of G. Here $Cl(G)$ is a Clar number of a benzenoid graph G and is equal to the size of the maximum cardinality resonant set of G. We generalized this theorem to any maximal resonant set of G, if G is an elementary benzenoid graph without nice coronenes. In addition to this, we present the connection between alternating sets of G and subgraphs of $R(G)$, that are maximal hypercubes.

In the next section we formally introduce the concepts and notations of this paper. The known results are presented in Section 3. Then new results concerning maximal resonant sets are in the first part of Section 4 and the new results about alternating sets are given in the second part of that section. We conclude with some open problems regarding this topic.

2 Preliminaries

Benzenoid graphs are 2-connected subgraphs of the hexagonal lattice such that every bounded face is a hexagon. If all vertices of a benzenoid graph lie on its perimeter, then G is said to be catacondensed; otherwise it is pericondensed. In Figure 1 we see a well known pericondensed benzenoid graph called *coronene*. We refer to [1] for more information about these graphs, especially for their chemical meaning as representation of benzenoid hydrocarbons.

A *matching* of a graph G is a set of independent edges of G. A matching is *perfect*, if it covers all vertices of G.

A hexagon h is M*-alternating* if the edges of h appear alternately in and off the perfect

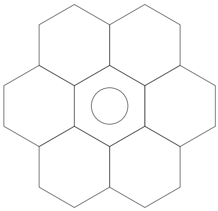

Figure 1: Coronene with a maximal resonant set.

matching M. An edge of a graph that has a perfect matching is *fixed* if it belongs to all or none of the perfect matchings of the graph. An *elementary* benzenoid graph is a benzenoid graph that has a perfect matching but no fixed edges. A benzenoid graph G is elementary if and only if there exists a perfect matching M of G such that the boundary of the outer face of G, a cycle, is M-alternating [12]. It is clear that every catacondensed benzenoid graph is elementary.

Let P be a set of hexagons of a benzenoid graph G. The subgraph of G obtained by deleting from G the vertices of the hexagons in P is denoted by $G - P$. It is clear that $G - P$ can be the empty graph.

Let P be a set of hexagons of a benzenoid graph G. Then the set P is called an *alternating set* of G if there exists such a perfect matching of G that contains a perfect matching of each hexagon in P. It is easy to see that if P is an alternating set of a benzenoid graph G, then $G - P$ is empty or has a perfect matching [13, 14]. An alternating set is *maximal* if it is not contained in another alternating set. An alternating set P of a benzenoid graph G satisfying $G - P$ is empty or has a unique perfect matching is called a *canonical* alternating set.

The *Fries number* of a benzenoid graph G with at least one perfect matching [15] is the maximum of the cardinalities over all alternating sets of G and is denoted by $Fr(G)$.

Let P be an alternating set of a benzenoid graph G. If the hexagons of P are pair-wise disjoint, then P is a *resonant set* [16, 17]. Alternatively [18, 19], P is a resonant set of G if the hexagons in P are pair-wise disjoint and there exists such a perfect matching of G that contains a perfect matching of each hexagon in P.

In figures, resonant sets are indicated with circles (see Figure 1 with the coronene and its maximal resonant set (which is not canonical) and alternating sets with filled circles (see Figure 2 for an example of alternating sets).

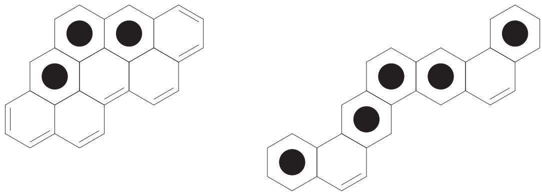

Figure 2: Maximal alternating sets of a pericondensed and a catacondensed benzenoid graph.

The *Clar number* of a benzenoid graph with at least one perfect matching [20] is the maximum of the cardinalities of all the resonant sets of G and is denoted by $Cl(G)$. A resonant set whose cardinality is the Clar number is called a *maximum cardinality* resonant set.

Let P be an alternating set of a benzenoid graph G. If there exists a perfect matching M of G such that M contains a perfect matching of each hexagon of P, than P is called an *M-alternating set* of G. Each hexagon of P is then a *M-alternating hexagon.* For every perfect matching M of a benzenoid graph G, there exists an M-alternating hexagon [22]. Consequently, P is called an *M-resonant set*, if hexagons of P are pair-wise disjoint (i.e. if P is a resonant set) [21]. It is clear that a set of hexagons P is resonant if and only if it is M-resonant for some perfect matching M.

The symmetric difference of two finite sets A and B is defined as $A \oplus B = (A \cup B) - (A \cap B)$. Let G be a benzenoid graph possessing at least one perfect matching. Then the vertex set of the *resonance graph* $R(G)$ of G consists of all perfect matchings of G, two vertices being adjacent whenever their symmetric difference forms the edge set of a hexagon of G.

A subgraph H of a graph G is said to be *nice* if $G - H$ admits a perfect matching.

Let the *distance* $d_G(u, v)$ between vertices u and v of a graph G be the usual shortest path distance, the index can be omitted if the considered graph is clear from the context. A subgraph H of a graph G is an *isometric* subgraph if $d_H(u, v) = d_G(u, v)$, for all $u, v \in V(H)$.

The *k-dimensional hypercube* Q_k, where k is a positive integer, is the graph whose vertex set is the set of all binary sequences of length k and two vertices are adjacent iff they differ in exactly one position. For our purposes we will consider a vertex as a 0-dimensional hypercube. A *partial cube* is an isometric subgraph of a hypercube [23, 24].

It is well known, that the set of edges of a partial cube whose end vertices differ in the i-th position and coincide in all others, form an equivalence class of the Djoković-Winkler's relation Θ [25, 23], where edges $e = uv$ and $f = xy$ of a graph G are in relation Θ, if

$$d_G(u, x) + d_G(v, y) \neq d_G(u, y) + d_G(v, x)\,.$$

Let v be a vertex of a graph G. Then the *degree* of v is $d(v) = |\{u; vu \in E(G)\}|$. The *maximum degree* of a graph G, $\Delta(G)$, is the maximum of degrees over all vertices of G.

3 Known results

For the clarity we will explicitly state the known results, that are of importance for us. In order to do that some preparation is needed.

Let G be a benzenoid graph with a perfect matching and $R(G)$ its resonance graph. Let H be a subgraph of $R(G)$ isomorphic to the k-dimensional hypercube for some positive integer k. We may assume that the vertices of H (considered as the vertices of $R(G)$) are labeled with the binary sequences of length k such that two vertices of H are adjacent if and only if their binary sequences differ in exactly one position. Consider the following vertices of H:

$$M \equiv \langle 000\ldots 0\rangle\,,\; M^1 \equiv \langle 100\ldots 0\rangle\,,\; M^2 \equiv \langle 010\ldots 0\rangle\,,\;\ldots,\; M^k \equiv \langle 000\ldots 1\rangle\;.$$

By the definition of the resonance graph, each of the edges MM^1, MM^2, $\ldots, MM^k$ corresponds to a unique hexagon of G. More precisely, for each $j = 1, 2, \ldots, k$, let h_j denote the symmetric difference of M and M^j. It was proved in [26] that, given arbitrary vertices M' and M'' of H whose binary sequences differ only at the j-th place for some $j \in \{1, 2, \ldots, k\}$, the symmetric difference of M' and M'' is the hexagon h_j. Moreover [26], the set $S_H = \{h_1, h_2, \ldots, h_k\}$ is a resonant set of G of cardinality k. Therefore, we call S_H the resonant set associated with a subgraph H of $R(G)$ isomorphic to a hypercube. Let us mention, that edges MM^j, $j = 1, 2, \ldots, k$, belong to different Θ-classes, since no two incident edges of a partial cube can be in the same Θ-class.

Let G be a benzenoid graph with a perfect matching and $R(G)$ its resonance graph. Let S be a resonant set of G of cardinality k for some positive integer k. If the subgraph $G - S$ is empty, let M be the empty set, otherwise, let M be a perfect matching of $G - S$. For each choice of M, the 2^k perfect matchings of the hexagons in S produce 2^k perfect matchings of G. It is clear that for each choice of M, the set of 2^k perfect matchings of G can be coded with integer sequences of length $k+1$ where the first integer in the sequence denotes the choice of M and the remaining k integers are binary digits. Hence, the subgraph of $R(G)$ induced by each such set of 2^k perfect matchings of G is isomorphic to a k-dimensional hypercube.

Thus, given a resonant set of G of cardinality k for some positive integer k this procedure associates a unique subgraph $R(G)$ isomorphic to the k-dimensional hypercube if S is a canonical resonant set, otherwise, it associates as many subgraphs of $R(G)$ isomorphic to the k-dimensional hypercube as the number of perfect matchings of $G-S$. This allows the definition of the set of subgraphs of $R(G)$ isomorphic to a hypercube associated with a resonant set. For a resonant set S, let us denote the associated set of hypercubes with $\mathcal{H}_S$.

Let G be a benzenoid graph with a perfect matching and $R(G)$ its resonance graph. Let $\mathcal{H}(R(G))$ be the set of subgraphs of $R(G)$ isomorphic to hypercubes and $\mathcal{S}(G)$ be the family of nonempty resonant sets of G. Then we can state the following theorems from [11].

Theorem 3.1. *[11] Let G be a benzenoid graph with a perfect matching and let $f : \mathcal{H}(R(G)) \to \mathcal{S}(G)$ be a mapping defined with $f(H) = S_H$ for $H \in \mathcal{H}(R(G))$. Then the inverse image of a nonempty resonant set S under the mapping f is $\mathcal{H}_S$.*

Note that Theorem 3.1 asserts that mapping f is surjective, a result first proved in [26].

Theorem 3.2. *[11] Let G be a benzenoid graph with a perfect matching. Then there exists a bijective mapping from the set of subgraphs of $R(G)$ isomorphic to the $Cl(G)$-dimensional hypercube into the family of maximum cardinality resonant sets of G.*

4 New results

4.1 $R(G)$ and maximal resonant sets of G

We will generalize Theorem 3.2 to the family of maximal resonant sets of an elementary benzenoid graph without nice coronenes. First we need the following lemma.

Lemma 4.1. *[27] Let G be an elementary benzenoid graph. Then G has no nice coronenes* *if and only if for any pair of disjoint cycles that form a nice subgraph of G their interiors are disjoint.*

Lemma 4.2. *Let G be an elementary benzenoid graph without nice coronenes. Then S is a maximal resonant set of G if and only if S is a canonical set of G.*

Proof. The only if part follows from [28].

For the if part let S be a maximal resonant set of G and suppose S is not canonical. Then $G-S$ allows at least two different perfect matchings. It follows that $G-S$ contains a cycle C which is an alternating cycle in both perfect matchings. Let $\overline{C}$ denote the cycle C together with its interior. We now consider two possibilities.

First assume that $S \cap \overline{C} = \emptyset$. Since C is an alternating cycle, $\overline{C}$ is an elementary benzenoid graph. Therefore $\overline{C}$ contains at least one alternating hexagon h [12, 16]. But then $S \cup \{h\}$ is also a resonant set which contradicts the maximality of S.

Assume now $S \cap \overline{C} \neq \emptyset$. Since $C \in G-S$, then there exists at least one such hexagon $h \in S$ that $h \in \overline{C}$, moreover C and h are disjoint and form a nice subgraph of G. By Lemma 4.1 graph G has a nice coronene what is, again, a contradiction. $\square$

Theorem 4.3. *Let G be an elementary benzenoid graph G without nice coronenes. Then there exists a bijective mapping from the set of subgraphs of $R(G)$ that are maximal hypercubes into the family of maximal resonant sets of G.*

Proof. Let H be a maximal hypercube of dimension k of the resonance graph $R(G)$. Then the image of H under the mapping f defined in Theorem 3.1 is a resonant set S of cardinality k. S must be a maximal resonant set, otherwise the inverse image of S under the mapping f is $\mathcal{H}_S$, where the hypercubes in $\mathcal{H}_S$ are of dimension greater than k, which is a contradiction, since $H \in \mathcal{H}_S$.

By Lemma 4.2 a maximal resonant set S of G is also a canonical resonant set. Hence, by Theorem 3.1 the inverse image of a maximum cardinality set under the mapping f defined in Theorem 3.1 is a singleton set containing a subgraph of $R(G)$ isomorphic to the k-dimensional hypercube. $\square$

Now we can assign to each maximal resonant set S of an elementary benzenoid graph G without nice coronenes a unique hypercube $H_S \subseteq R(G)$ of dimension $|S|$. For a pericondensed benzenoid graph from Figure 3 we have eight maximal resonant sets, one of them has cardinality one, six have cardinality two and there is one maximum cardinality resonant set $\{h_3, h_5, h_7\}$. Therefore in the resonance graph $R(G)$ we have eight maximal hypercubes, where six of them are 2-dimensional and then we have one 3-dimensional and one 1-dimensional hypercube. For example, for a maximal resonant set $S = \{h_2, h_7\}$ the corresponding maximal hypercube $H_S \subseteq R(G)$ is a 2-dimensional hypercube, induced with edges from Θ-classes E_{h_2}, E_{h_7} (for the clarity of figures an edge of $R(G)$ from the Θ-class E_{h_i} is denoted with i).

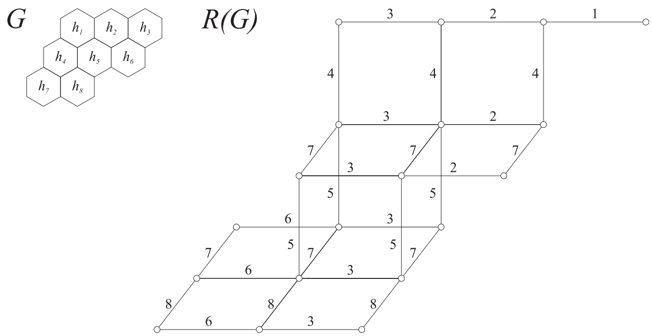

Figure 3: The resonance graph $R(G)$ of a benzenoid graph G.

4.2 $R(G)$ and alternating sets of G

We are interested in a connection between different maximal hypercubes of the resonance graph of a benzenoid graph G. In order to explain it we need to consider the alternating sets of G.

Theorem 4.4. *Let G be a benzenoid graph without nice coronenes and $R(G)$ its resonance graph. Then a vertex $M \in R(G)$ is incident with vertices $M_1, M_2, \ldots, M_k$, where $M \oplus M_i = h_i$, for $i = 1, 2, \ldots, k$, if and only if $P = \{h_1, h_2, \ldots, h_k\}$ is an M-alternating set of G.*

Proof. Let M be a vertex of a resonance graph $R(G)$ and let $M_1, M_2, \ldots, M_k$ be incident vertices of M in $R(G)$. By the definition of the resonance graph, a symmetric difference $M \oplus M_i$ is a hexagon h_i of G, where $i = 1, 2, \ldots, k$. Since $R(G)$ is a partial cube [10], no two incident edges belong to the same Θ-class and hexagons $h_1, h_2, \ldots h_k$ are all distinct. Further, they are all M-alternating hexagons and we have an alternating set.

For the converse, let P be an alternating set of G and M such a perfect matching, that every hexagon in P is M-alternating set. Let h be a hexagon of P. Since h is M-alternating, there exists a perfect matching M' such, that $M \oplus M' = h$ and therefore MM' is an edge in $R(G)$. By the same conclusion as above, different hexagons of P induce different edges incident with M. $\square$

Corollary 4.5. *Let G be a benzenoid graph without nice coronenes. The maximum degree of a vertex in $R(G)$ equals the size of a maximum cardinality alternating set of G.*

Proof. Let P be a maximum cardinality alternating set of G. From Theorem 4.4 there exists such a vertex M in the resonance graph $R(G)$ that the degree of M is $|P|$. Following the same line of thought as in the proof of Theorem 4.4 we can see that the existence of a vertex with a larger degree would be a contradiction to the maximum cardinality of P. $\square$

From the definition of the Fries number the next corollary immediately follows.

Corollary 4.6. *Let G be a benzenoid graph without nice coronenes. The Fries number of G is the maximum degree of the resonance graph $R(G)$*

$$Fr(G) = \Delta(R(G)) .$$

Let P be a maximal alternating set and let $[P] \subseteq G$ be a graph, induced with vertices of hexagons from P. Let $\mathcal{M}$ be the set of such perfect matchings of G, that for any $M \in \mathcal{M}$ all the hexagons in P are M-alternating. First we observe, that the connected components of $[P]$ must be catacondensed benzenoid graphs, since the hexagons of a pericondesed benzenoid graph can not be simultaneously alternating.

Let the number of hexagons in a connected component of $[P]$ be a *size* of the component. If a component of $[P]$ has the size greater then one, then perfect matchings from $\mathcal{M}$ restricted to that component, are identical. On the other hand, if the component is of size one, t.i. a *single* hexagon, say h, then for any $M \in \mathcal{M}$ there exists $M' \in \mathcal{M}$ such, that $M \oplus M' = h$. Since any maximal alternating set of a benzenoid graph is canonical ([13]), we can conclude that if $[P]$ has k components of size one, t.i. single hexagons, then $|\mathcal{M}| = 2^k$.

By the same argument as in Section 3, where we considered resonant sets, the subgraph in $R(G)$ induced with perfect matchings from $\mathcal{M}$ is isomorphic to the k-dimensional hypercube. So, to any maximal alternating set $P \subseteq G$ we can associate a unique hypercube H_P in $R(G)$. If $h_1, h_2, \ldots, h_k$ are single hexagons of P, then H_P is spanned with edges from Θ-classes $E_{h_1}, E_{h_2}, \ldots, E_{h_k}$ of $R(G)$. All the vertices of H_P are therefore incident with edges from Θ-classes $E_{h_1}, E_{h_2}, \ldots, E_{h_k}$ as well as with edges from any Θ-class E_{h_j}, where hexagon h_j is in P and is not a single hexagon (t.i. $j \neq 1, 2, \ldots, k$). Let us mention, if there are no single hexagons in P, then H_P is a hypercube of dimension 0, that is a vertex.

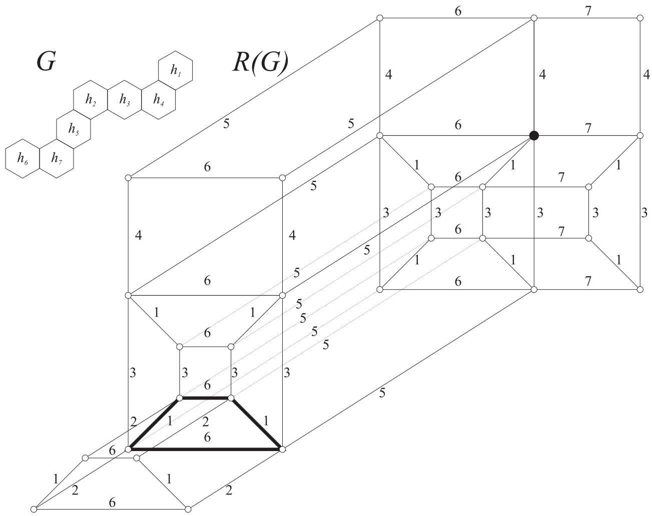

Figure 4: The resonance graph $R(G)$ of a benzenoid graph G and two hypercubes $H_P \subset R(G)$.

In Figure 4 we have an example of a catacondensed benzenoid graph G together with its resonance graph $R(G)$, where for a maximal alternating set $P_1 = \{h_1, h_2, h_3, h_5, h_6\}$ the associated hypercube H_{P_1} of dimension two is highlighted, and for a second maximal alternating set $P_2 = \{h_1, h_3, h_4, h_5, h_6, h_7\}$ the associated hypercube H_{P_2} is a vertex, marked with a black circle on Figure 4, and is incident with edges from Θ-classes $E_{h_1}, E_{h_3}, E_{h_4}, E_{h_5}, E_{h_6}, E_{h_7}$ (as in Figure 3 edges from Θ-class E_{h_i} are labeled with i).

Theorem 4.7. *Let G be an elementary benzenoid graph without nice coronenes. Let P be a maximal alternating set and S a maximal resonant set of G, and let H_P and H_S be the associated hypercubes in $R(G)$, respectively. Then $S \subseteq P$ if and only if $H_P \subseteq H_S$.*

Proof. Let $P = \{h_1, h_2, \ldots, h_k\}$ be a maximal alternating set and further let $S = \{h_{s_1}, h_{s_2}, \ldots, h_{s_i}\}$ be a maximal resonant set, such that $S \subseteq P$. Let M be a vertex of the hypercube H_P. Then $d(M) = k$ and the incident edges of M belong to distinct Θ-classes $E_{h_1}, E_{h_2}, \ldots, E_{h_k}$. Since the hypercube H_S is spanned with edges from Θ-classes $E_{h_{s_1}}, E_{h_{s_2}}, \ldots, E_{h_{s_i}}$ and S is a maximal resonant set, by Theorem 4.3 the hypercube H_S is uniquely determined and the vertex M must belong to H_S.

If at least one of the hexagons from P is a single hexagon, then H_P is not a vertex. Considering this, let MM' be an edge of the hypercube H_P. We have just shown that $M, M' \in V(H_S)$. Suppose $MM' \notin E(H_S)$. Since MM' is an edge of H_P, the symmetric difference $M \oplus M' = h$, where h is a single hexagon of P and by our assumption, $h \notin S$, which is a contradiction with the maximality of S.

For the only if part, suppose $H_P \subseteq H_S$. Let M be a vertex of H_P and let h be an arbitrary hexagon of S. Then $M \in V(H_S)$ and since every vertex of H_S is incident with an edge from the Θ-class E_h, the vertex M is also incident with an edge from E_h. Therefore h must belong to P. Since h was arbitrarily chosen it follows that $S \subseteq P$.

□

Corollary 4.8. *Let G be an elementary benzenoid graph without nice coronenes, with P being a maximal alternating set of G and let S be the union of all maximal resonant sets of $[P]$. Then $S = P$.*

Proof. Since every maximal resonant set of $[P]$ is also a maximal resonant set of G, the corollary follows immediately from the proof of Theorem 4.7.

□

5 Open problems

1. Theorem 4.3 holds also in the case of any benzenoid graph without nice coronenes.

2. Let $\mathcal{H}$ be a set of all maximal hypercubes of an elementary benzenoid graph G without nice coronenes. The question is, Can the resonance graph $R(G)$ be composed from the elements of $\mathcal{H}$ with the additional information on the adjacency of hexagons without computing 1-factors?

References

[1] I. Gutman, S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer, Berlin, 1989.

[2] M. Randić, Resonance in catacondensed benzenoid hydrocarbons, *Int. J. Quantum Chem.* **63** (1996) 585–600.

[3] F. Zhang, X. Guo, R. Chen, Z–transformation graphs of perfect matchings of hexagonal systems, *Discr. Math.* **72** (1988) 405–415.

[4] W. Gründler, Mesomerie und Quantenmechanik, *Z. Chem. (Leipzig)* **23** (1983) 157–167.

[5] S. El–Basil, Kekulé structures as graph generators, *J. Math. Chem.* **14** (1993) 305–318.

[6] S. El–Basil, Generation of lattice graphs. An equivalence relation on Kekulé counts of catacondensed benzenoid hydrocarbons, *J. Mol. Struct. (Theochem)* **288** (1993) 67–84.

[7] R. Chen, F. Zhang, Hamilton paths in Z–transformation graphs of perfect matchings of hexagonal systems, *Discr. Appl. Math.* **74** (1997) 191–196.

[8] F. Zhang, X. Guo, R. Chen, The connectivity of Z–transformation graphs of perfect matchings of hexagonal systems, *Acta Math. Appl. Sinica* **4** (1988) 131–135.

[9] H. Zhang, Z–transformation graphs of perfect matchings of plane bipartite graphs: A survey, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 457–476.

[10] H. Zhang, P. C. B. Lam, W. C. Shiu, Resonance graphs and a binary coding for the 1–factors of benzenoid systems, *SIAM J. Discr. Math.* **22** (2008) 971–984.

[11] K. Salem, S. Klavžar, A. Vesel, P. Žigert, The Clar formulas of a benzenoid system and the resonance graph, *Discr. Appl. Math.* **157** (2009) 2565–2569.

[12] F. Zhang, R. Chen, When each hexagon of a hexagonal system covers it, *Discr. Appl. Math.* **30** (1991) 63–75.

[13] K. Salem, H. Abeledo, A maximal alternating set of a hexagonal system, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 159–176.

[14] K. Salem, I. Gutman, The unfixed subgraph of a catacondensed hexagonal system obtained by fixing an alternating set, *J. Math. Chem.* **38** (2005) 503–510.

[15] P. Hansen, M. Zheng, Numerical bonds for the perfect matching vectors of a polyhex, *J. Chem. Inf. Comput. Sci.* **34** (1994) 305–308.

[16] I. Gutman, Topological properties of benzenoid systems. XIX. Contributions to the aromatic sextet theory, *Wiss. Z. Thechn. Hochsch. Ilmenau* **29** (1983) 57–65.

[17] H. Hosoya, T. Yamaguchi, Sextet polynomial. A new enumeration and proof technique for the resonance energy applied to the aromatic hydrocarbons, *Tetrahedron Lett.* **52** (1975) 4659–4662.

[18] H. Abeledo, G. Atkinson, The Clar and Fries problems for benzenoid hydrocarbons are linear programs, in: P. Hansen, P. Fowler, M. Zheng (Eds.), *Discrete Mathematical Chemistry*, Am. Math. Soc., Providence, 2000, pp. 1–8.

[19] H. Abeledo, G. Atkinson, Unimodularity of the Clar number problem, *Lin. Algebra Appl.* **420** (2007) 441–448.

[20] P. Hansen, M. L. Zheng, Upper bounds for the Clar number of a benzenoid hydrocarbon, *J. Chem. Soc. Faraday Trans.* **88** (1992) 1621–1625.

[21] K. Salem, Towards a combinatorial efficient algorithm to solve the Clar problem of benzenoid hydrocarbons, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 419–426.

[22] I. Gutman, Covering hexagonal systems with hexagons, in: *Proceedings of the Fourth Yugoslav Seminar on Graph Theory*, Univ. Novi Sad, Novi Sad, 1983, pp. 151–160.

[23] P. Winkler, Isometric embeddings in products of complete graphs, *Discr. Appl. Math.* **7** (1984) 221–225.

[24] S. Klavžar, H. M. Mulder, Partial cubes and crossing graphs, *SIAM J. Discr. Math.* **15** (2002) 235–251.

[25] D. Djoković, Distance preserving subgraphs of hypercubes, *J. Combin. Theory Ser. B* **14** (1973) 263–267.

[26] K. Salem, S. Klavžar, I. Gutman, On the role of hypercubes in the resonance graphs of benzenoid graphs, *Discr. Math.* **306** (2006) 699–704.

[27] F. Zheng, R. Chen, A theorem concerning polyhex graphs, *MATCH Commun. Math. Comput. Chem.* **19** (1986) 176–188.

[28] S. Klavžar, K. Salem, A. Taranenko, Maximum cardinality resonant sets and maximal alternating sets of hexagonal systems, *Comput. Math. Appl.* **59** (2010) 506–513.