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On dissection of graphs*

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Abstract

For a graph G, the dissection of G, denoted by $D(G)$, is a binary vector (x, y) introduced by Randic in 1979. Let $D(G) = (a(G), b(G))$. In this paper, we obtain the dissection of some special graphs. For a graph G and an edge $e \in E(G)$, we show that $b(G - e) < b(G)$. Moreover, if G is connected, for any induced proper subgraph H of G, $a(H) < a(G)$ with some exception. We also show that among all trees of order $n \geq 5$, the path P_n has the minimum $a(G)$ and $b(G)$, and the star $K_{1,n-1}$ has the maximum $a(G)$ and $b(G)$. Finally we prove that, for any tree T of order n, $a(T) > b(T)$ except for $T \cong P_n$ when $a(P_n) = b(P_n)$.

1 Introduction

The dissection of a graph was first introduced by Randic [3] in 1979, and was further investigated in [6]. For a graph $G = (V(G), E(G))$, the dissection of G, denoted by $D(G)$, is a binary vector (x, y) defined recursively as follows:

(1) If $G = K_1$, $D(G) = (1, 0)$.

(2) If $G = K_2$, $D(G) = (0, 1)$.

(3) If G is not connected, then $D(G) = \sum_{i=1}^{r} D(G_i)$, where $G_1, G_2, \cdots, G_r$ are all the components of G. If G is a connected graph of order $n \geq 3$, $D(G) = \sum_{v \in V(G)} D(G - v)$.

We denote the first and the second entry of the dissection $D(G) = (x, y)$ by $a(G)$ and $b(G)$ respectively. Namely, $a(G) = x$ and $b(G) = y$.

The dissection of graphs is a useful molecule descriptor of chemical molecular graphs. It was shown in [5] that the dissection parameters a and b produce good regression for steric factor of alkanes and correlate quite well with the hyper-Wiener index. From the obtained value of the dissection parameters of smaller trees, we can see that the novel parameters, which are integer, are very sensitive to molecular branching (see Table 1).

There are several graph invariants of a very high-resolution power [2, 4] that may be of interest for graph isomorphism testing. An interesting conjecture on dissection of graphs can be find in [5]: for two trees T_1 and T_2, $D(T_1) = D(T_2)$ if and only if $T_1 \cong T_2$. But it is not the subject of the present study.

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Table1: The dissection parameters for the smaller alkanes

Hexanes		Octanes	
n-hehexane	(54,54)	n-octane	(486,486)
2-methyl	(78,68)	2-methyl	(702,662)
3-methyl	(85,74)	3-methyl	(850,786)
2,3-eimethyl	(112,88)	4-methyl	(905,830)
2,2-dimethyl	(131,94)	2,5-dimethyl	(1014,914)
		3-ethyl	(1072,974)
Heptanes		2,4-dimethyl	(1241,1096)
n-heptane	(162,162)	2,2-dimethyl	(1314,1106)
2-methyl	(234,214)	2,3-dimethyl	(1340,1170)
3-methyl	(272,245)	3,4-dimethyl	(1526,1320)
3-ethyl	(312,279)	2-methyl-3-ethyl	(1600,1384)
2,4-dimethyl	(338,288)	3,3-dimethyl	(1693,1388)
2,3-dimethyl	(398,334)	2,2,4-trimethyl	(1919,1564)
2,2-dimethyl	(420,331)	3-methyl-3-ethyl	(2035,1644)
3,3-dimethyl	(488,380)	2,3,4-trimethyl	(1991,1670)
2,2,3-trimethyl	(614,460)	2,2,3-trimethyl	(2379,1900)
		2,3,3-trimethyl	(2531,2000)
		2,2,3,3; tetramethyl	(3708,2772)

In section 2, the dissection of some special graphs are given, and one will find that $a(G)$ and $b(G)$ are generally large numbers with contrast to the order of G. In section 3, we show for a graph G and an edge $e \in E(G)$, $b(G-e) < b(G)$, and if G is connected, for any induced proper subgraph H of G, $a(H) < a(G)$ with some exception. In section 4, we will see that both $a(G)$ and $b(G)$ increase with molecular branching when G is a tree and for any tree T of order n we have $a(T) > b(T)$ except for $T \cong P_n$.

For a graph $G = (V(G), E(G))$, $|V(G)|$ is called the order of G. If the order of G is equal to 1, G is called trivial, and nontrivial, otherwise. If $E(G) = \emptyset$, G is called an empty graph. For $v \in V(G)$ and $e \in E(G)$, let $G - e$ denote the graph obtained from G by deleting e, $G - v$ the graph obtained from G by deleting v and its incident edges. v is said to be a cut vertex if $G - v$ is not connected.

The complement of G, denoted by $\overline{G}$, is the graph with the same vertex set as G, but where two vertices are adjacent if and only if they are not adjacent in G. As usual, P_n, C_n and K_n are respectively, the path, cycle, and complete graph of order n. For two positive integers r and s, $K_{r,s}$ is the complete bipartite graph with two partite sets containing r and s vertices. In particular, $K_{1,s}$ is called a star. K_n^- denotes the graph resulting from K_n by deleting an edge. A graph T is called tree if it is connected and contains no cycle. We say two graphs G and H are disjoint if they have no vertex in common, and denote their union by $G + H$; it is called the disjoint union of G and H. The disjoint union of k copies of G is written as kG. Undefined terminologies and notation can be found in [1].

2 Dissections of some special graphs

In this section we get the dissections of K_n, K_n^-, P_n, C_n and $K_{m,n}$.

Proposition 2.1. For $n \geq 2$,

$$D(K_n) = (0, \frac{n!}{2}), \qquad D(K_n^-) = (n-2)!(2, \frac{(n+1)(n-2)}{2}).$$

Proof. Let $v_1, v_2, \cdots, v_n$ be all the vertices of K_n. By the definition,

$$\begin{aligned} D(K_n) &= \sum_{i=1}^{n} D(K_n - v_i) \\ &= nD(K_{n-1}) = n(n-1)D(K_{n-2}) = \cdots \\ &= n(n-1)\cdots 3D(K_2) \\ &= (0, \frac{n!}{2}). \end{aligned}$$

We prove (2) by induction on n. For $n = 2$, the result is trivial.

$$\begin{aligned} D(K_n^-) &= 2D(K_{n-1}) + (n-2)D(K_{n-1}^-) \\ &= 2 \times (0, \frac{(n-1)!}{2}) + (n-2) \times (n-3)!(2, \frac{n(n-3)}{2}) \\ &= ((n-2)! \times 2, (n-2)! \times [(n-1) + \frac{n(n-3)}{2}] \\ &= (n-2)!(2, \frac{(n+1)(n-2)}{2})). \quad \square \end{aligned}$$

Proposition 2.2. For $n \geq 3$, $D(P_n) = (2 \times 3^{n-3}, 2 \times 3^{n-3})$, $D(C_n) = (2n3^{n-4}, 2n3^{n-4})$.

Proof. We prove by induction on n. For $n = 3$, $D(P_3) = (2, 2)$ and the result holds. Now suppose $n \geq 4$ and the result is true for all paths of order less than n. Let $V(P_n) = \{v_1, v_2, \cdots, v_n\}$ and $E(P_n) = \{v_i v_{i+1}, i = 1, \cdots, n-1\}$. Then

$$\begin{aligned} D(P_n) &= D(P_n - v_1) + D(P_n - v_n) + \sum_{i=2}^{n-1} D(P_n - v_i) \\ &= 2D(P_{n-1}) + \sum_{i=2}^{n-1} (D(P_{i-1}) + D(P_{n-i})) \\ &= (2 \times 3^{n-4}, 2 \times 3^{n-4}) + \sum_{i=2}^{n-1} [(2 \times 3^{i-4}, 2 \times 3^{i-4}) + (2 \times 3^{n-i-1}, 2 \times 3^{n-i-1})] \\ &= (2 \times 3^{n-3}, 2 \times 3^{n-3}). \end{aligned}$$

Since $D(C_n) = nP_{n-1}$, the result follows. $\square$

Proposition 2.3. For any two positive integers m and n,

$$a(K_{m,n}) = n \sum_{i=2}^{m} (n+m-i-1)! \binom{m}{i} i + m \sum_{j=2}^{n} (n+m-j-1)! \binom{n}{j} j$$

$$b(K_{m,n}) = (m+n-2)! \cdot mn.$$

In Particular, $D(K_{1,n}) = (n! \sum_{k=1}^{n-1} \frac{1}{k!}, \quad n!)$.

Proof. Our proof is by induction on $m+n$. For $m+n = 3$, $K_{m,n} \cong K_{1,2} \cong P_3$, $D(K_{1,2}) = (2, 2)$, the result is true. Now let $m + n > 3$. It is easy to see that $D(K_{m,n}) = mD(K_{m-1,n}) + nD(K_{m,n-1})$, and thus by the induction hypothesis,

$$a(K_{m-1,n}) = n \sum_{i=2}^{m-1} (n+m-1-i-1)! \binom{m-1}{i} i + (m-1) \sum_{j=2}^{n} (n+m-1-j-1)! \binom{n}{j} j,$$

$$a(K_{m,n-1}) = (n-1)\sum_{i=2}^{m}(n+m-1-i-1)!\binom{m}{i}i + m\sum_{j=2}^{n-1}(n+m-1-j-1)!\binom{n-1}{j}j,$$

$$b(K_{m-1,n}) = (m+n-3)!\cdot(m-1)n \quad and \quad b(K_{m,n-1}) = (m+n-3)!\cdot m(n-1).$$

So we obtain

$$\begin{aligned} a(K_{m,n}) &= ma(K_{m-1,n}) + na(K_{m,n-1}) \\ &= n\sum_{i=2}^{m}(n+m-i-1)!\binom{m}{i}i + m\sum_{j=2}^{n}(n+m-j-1)!\binom{n}{j}j. \\ b(K_{m,n}) &= mb(K_{m-1,n}) + nb(K_{m,n-1}) \\ &= m[(m+n-3)!\cdot(m-1)n] + n[(m+n-3)!\cdot m(n-1)] \\ &= (m+n-2)!\cdot mn \quad \square \end{aligned}$$

3 Dissection of a graph and its subgraph

Theorem 3.1. For a graph G and its any subgraph H, we have $b(G) \geq b(H)$, with equality if and only if $E(G) = E(H)$.

Proof. If G is an empty graph, then the result is trivial. So assume that G is not empty, and it is enough to show that for each $e \in E(G)$ of a graph G, $b(G-e) < b(G)$. We prove by induction on the order n of G. For $n = 2$, the result is true. Now assume that $n \geq 3$ and $e \in E(G)$. If G is not connected, denote all the component of G by $G_1, G_2, \cdots, G_k$. Without loss of generality, suppose $e \in E(G_1)$. By the induction hypothesis, $b(G_1 - e) < b(G_1)$. Thus $b(G-e) = b(G_1-e) + b(G_2) + \cdots + b(G_k) < b(G_1) + b(G_2) + \cdots + b(G_k) = b(G)$. Now suppose G is connected. Since G has order at least three, there is a vertex w, say, which is not incident with e in G. Since $b(G-e-v) = b(G-v-e)$, by the induction hypothesis, for any $v \in V(G)$, $b(G-e-v) \leq b(G-v)$ and $b(G-e-w) < b(G-w)$. Consequently, from $b(G) = \sum_{v\in V(G)} b(G-v)$ and $b(G_e) = \sum_{v\in V(G)} b(G_e - v)$, we have $b(G-e) < b(G)$. $\square$

As an immediate corollary we have

Corollary 3.2. For any graph G of order n, we have $0 \leq b(G) \leq \frac{n!}{2}$, with the left-hand side equality if and only if $G \cong \overline{K_n}$ and with the right-hand side equality if and only if $G \cong K_n$.

Theorem 3.3. For any graph G, $a(G) = 0$ if and only if each component of G is a complete graph of order at least two.

Proof. If each component of G is a complete graph of order at least two, then $a(G) = 0$. We prove the necessity by induction on the order n of G. For $n = 2$ and $n = 3$, the result is trivial. Now suppose $n \geq 4$ and the result holds for all graphs of order less than n. If G is not connected, then by the induction hypothesis each component of G is a complete graph of order at least two, the result follows. Next assume that G is connected and we will prove that G is a complete graph. Since $a(G) = \sum_{v\in V(G)} a(G-v) = 0$, for any vertex $v \in V(G)$, $a(G-v) = 0$ and thus $a(G-v)$ is composed of complete graphs of order at least two. Since G is connected, it contains two non-cut vertices v_1 and v_2. Then $G-v_1$ and $G-v_2$ are connected, and thus are the complete graph of order $n-1$ by the induction hypothesis. It follows that for any $v \in V(G)\backslash\{v_1, v_2\}$, $G-v$ is connected and is a complete graph of order $n-1$, and thus G must be a complete graph. $\square$

Theorem 3.4. Let G be a connected graph of order $n \geq 3$. Then there is a vertex v such that $a(G-v) = a(G)$ if and only if $G \cong K_n$ or $G \cong P_3$.

Proof. If $G \cong K_n$ and $v \in V(G)$ or $G \cong P_3$ and v is the vertex of degree 2, then $a(G-v) = a(G)$. Next we show the necessity. Assume G is a connected graph with a vertex $v \in V(G)$ such that $a(G-v) = a(G)$. Further we assume that G is not a complete graph, so it suffices to prove that $G \cong P_3$. Moreover, since P_3 is the only connected graph of order 3 which is not a complete graph, we need only verify $n = 3$. From $D(G) = \sum_{v \in V(G)} D(G-v)$ and Theorem 3.3, $a(G-v) = a(G) > 0$ and for any vertex $u \in V(G) \setminus \{v\}$, $a(G-u) = 0$, thus $G-u$ is composed of complete graphs of order at least 2. Since G is connected, it contains at least two non-cut vertices. Let u_1 be a non-cut vertex different from v. Then $G - u_1 \cong K_{n-1}$. If $n > 3$, we can find second non-cut vertex u_2, say, from $V(G) \setminus \{u_1, v\}$. Again $G - u_2 \cong K_{n-1}$. Now choose an arbitrary vertex $u_3 \in V(G) \setminus \{v, u_1, u_2\}$. It is clear that u_3 is neither a cut vertex. It implies that G is a complete graph, a contradiction. So, $n = 3$ and the proof is complete. □

Both Proposition 2.1 and Theorem 3.3 tell us that the parameter $a(G)$ has no monotone property for subgraph relation as $b(G)$ does. But we have

Theorem 3.5. Suppose G is a connected graph of order n and H is an induced subgraph of G. Then $a(G) > a(H)$ unless $G \cong K_n$, or $G \cong P_3$ and $H \cong \overline{K_2}$.

Proof. It suffices to show that

$$a(G) \leq a(H) \text{ if and only if } G \cong K_n, \text{ or } G \cong P_3 \text{ and } H \cong \overline{K_2} \quad (1).$$

The sufficiency of (1) is obvious. Next we prove the necessity of (1) by induction on the order n of G. Suppose G is a connected graph with an induced subgraph H of G such that $a(H) \geq a(G)$. Further we assume that G is not a complete graph, so it suffices to prove that $G \cong P_3$.

First let us consider the case $n = 3$. Since G is connected and $G \ncong K_3$, $G \cong P_3$, and thus $H \in \{K_1, K_2, \overline{K_2}\}$. By $a(H) \leq 2 = a(P_3) = a(G)$, $H \cong \overline{K_2}$, (1) holds. Next we show that there is no graph G of order $n \geq 4$ having the desired property. Since G is not complete graph, by Theorem 3.4, for any $v \in V(G)$, $a(G) > a(G-v)$, and since $a(H) > a(G)$, we have $a(H) > a(G-v)$ and thus $|V(H)| \leq n-2$.

Claim 1. G has a non-cut vertex u in $V(G) \setminus V(H)$.

By contradiction, suppose each vertex in $V(G) \setminus V(H)$ is a cut vertex and we take a vertex v_0 from it. Then $G - v_0$ is not connected, and denote all the components of $G - v_0$ by $G_1, G_2, \cdots, G_k$. Let $H_i = H \cap G_i$ for each $i = 1, \cdots, k$. Since $a(G - v_0) = a(G_1) + a(G_2) + \cdots + a(G_k)$, $a(H) = a(H_1) + a(H_2) + \cdots + a(H_k)$ and $a(H) > a(G - v_0)$, we have $a(H_1) > a(G_1)$, without loss of generality. By the induction hypothesis, G_1 is a complete graph of order at least two and H_1 is the trivial graph. Moreover, we claim that $G_1 \cong K_2$. Otherwise, one can easily find a vertex from $V(G_1) \setminus V(H)$, which is not a cut vertex of G. It contradicts with our assumption. Hence set $V(G_1) = \{v_1, v_1'\}$, where $v_1 \in V(G) \setminus V(H)$ and $v_1' \in V(H)$. Since v_1 is a cut vertex, $G - v_1$ is not connected and has exactly two components, one of which is the isolated vertex v_1' and the other, denoted by F, containing v_0. Again by Theorem 3.4, $a(G) > a(G - v_1) = a(F) + 1$, and combining this with $a(H) = a(H \cap F) + 1$ and $a(H) \geq a(G)$, we have $a(H \cap F) > a(F)$. So by the induction hypothesis, F is a complete graph of order at least two and $F \cap H$ is also the trivial graph (an isolated vertex). By changing the role of v_0 to v_1, we also have $F \cong K_2$. Thus $G \cong P_4$. However, we have seen in Proposition 2.3 that $a(P_4) = 6$ and $a(H) \leq 2$. A contradiction. This shows the claim.

By Claim 1, $G - u$ is connected, and H is the subgraph of $G - u$ with $a(H) > a(G - u)$. By the induction hypothesis, $G - u$ ia a complete graph and $H \cong K_1$. Since $a(G) < a(H) = 1$, G must be a complete graph by Theorem 3.3, a contradiction. This completes the proof. □

Note that the condition of connectedness for G in Theorem 3.5 cannot be omitted. Let us consider $G = K_2 + 2K_1$. Clearly, G has an induced subgraph $H \cong 3K_1$. However, $a(G) = 2 < 3 = a(H)$. Also, from Theorem 3.5, we have more by strengthening Theorem 3.4 as follows.

Corollary 3.6. Suppose G is a connected graph of order n and H is an induced subgraph of G. Then

(1) $a(G) = a(H)$ if and only if both G and H are complete graphs of order at least two, or $G \cong P_3$ and $H \cong \overline{K_2}$.

(2) $a(G) < a(H)$ if and only if $G \cong K_n$ with $n \geq 2$ and $H \cong K_1$.

4 Dissection of trees

Lemma 4.1. Let G_1 and G_2 be two nontrivial vertex-disjoint connected graphs. Suppose $u_i \in V(G_i)$ for $i = 1, 2$ and G is obtained from G_1 and G_2 by joining u_1 and u_2. Then $a(G) > a(G_1) + a(G_2)$ and $b(G) > b(G_1) + b(G_2)$.

Proof. Take a vertex $u \in V(G) \setminus \{u_1, u_2\}$. Then the component of $G - u$ containing u_1 (or u_2) is not a complete graph. By Theorem 3.3, $a(G - u) > 0$. Therefore,

$$\begin{aligned} a(G) &\geq a(G-u_1) + a(G-u_2) + a(G-u) \\ &= (a(G_1-u_1) + a(G_2)) + (a(G_2-u_2) + a(G_1) + a(G-u) \\ &> a(G_1) + a(G_2). \end{aligned}$$

By Theorem 3.1, $b(G) > b(G - u_1u_2) = b(G_1) + b(G_2)$. □

Lemma 4.2. Suppose G_1 and G_2 are two nontrivial vertex-disjoint connected graphs, $u_i \in V(G_i)$ for $i = 1, 2$. Let G is obtained from G_1 and G_2 by identifying u_1 and u_2 as u. Then

(1) $a(G) > a(G_1) + a(G_2)$;

(2) $b(G) \geq b(G_1) + b(G_2)$, with equality if and only if $G_1 \cong G_2 \cong K_2$.

Proof. Let n_i be the number of vertices of G_i. By induction on $n_1 + n_2$. First assume that $min\{n_1, n_2\} = 2$, without loss of generality, let $n_1 = 2$ and $u_1' = V(G_1) \setminus \{u_1\}$. Then $a(G) \geq a(G_1 - u_1') + a(G - u_1) \geq a(G_2) + 1 > a(G_1) + a(G_2)$. In particular, if $n_1 = n_2 = 2$ then $G_1 \cong G_2 \cong K_2$, and thus $G \cong P_3$. So $a(G) = 2 > 0 = a(G_1) + a(G_2)$, and $b(G) = 2 = b(G_1) + b(G_2)$.

Now assume $min\{n_1, n_2\} \geq 3$, and the result hold for any pair of graphs with the sum of their orders less than $n_1 + n_2$. Let $w_i \in V(G_i) \setminus \{u_i\}$ be not a cut vertex of $G_i - w_i$ for $i = 1, 2$. Then $G_i - w_i$ is connected, and $G - w_i$ connected. Hence, by the induction hypothesis, $a(G - w_1) > a(G_1 - w_1) + a(G_2)$ and $a(G - w_2) > a(G_2 - w_2) + a(G_1)$. Therefore,

$$\begin{aligned} a(G) &\geq a(G-w_1) + a(G-w_2) \\ &> a(G_1) + a(G_2) + a(G_1-w_1) + a(G_2-w_2) \\ &> a(G_1) + a(G_2). \end{aligned}$$

Since at least one of $G_1 - w_1$ and $G_2 - w_2$ is nontrivial, by Corollary 3.2, $b(G_1 - w_1) + b(G_2 - w_2) > 0$. Therefore,

$$b(G) \geq b(G-w_1) + b(G-w_2) > b(G_1) + b(G_2) + b(G_1-w_1) + b(G_2-w_2) > b(G_1) + b(G_2).$$

One also can see that $b(G) = b(G_1) + b(G_2)$ if and only if $G_1 \cong G_2 \cong K_2$. □

Lemma 4.3. Suppose G_1 and G_2 are two nontrivial vertex-disjoint connected graphs, $u_i \in V(G_i)$ for $i = 1, 2$. Let G be a graph obtained from G_1 and G_2 by joining u_1 and u_2, G' be the graph obtained from G_1 and G_2 by identifying u_1 and u_2 as vertex u and adding a new vertex w joining to u. Then

(1) $a(G') > a(G)$;

(2) $b(G') \geq b(G)$, with equality if and only if $G_1 \cong G_2 \cong K_2$.

Proof. Let $n_i = |V(G_i)|$ for $i = 1, 2$. By induction on $n_1 + n_2$. If $n_1 = n_2 = 2$, $G' = K_{1,3}$ and $G \cong P_4$. By Propositions 2.2 and 2.3, $D(G') = (9, 6)$ and $D(G) = (6, 6)$, thus result holds. Now suppose $n_1 + n_2 \geq 5$.

We claim that for any vertex $v \in V(G) \setminus \{u_1, u_2\}$, $a(G' - v) \geq a(G - v)$. To see this, suppose $v \in V(G_1)$ and denote all the components of $G - v$ by $H_1, H_2, \cdots, H_k$, where H_1 is the component containing u_1 and u_2. Then $H_1', H_2, \cdots, H_{k-1}, H_k$ be those of $G' - v$, where H_1' is the one containing u. So it is enough to show that $a(H_1') \geq a(H_1)$. Note that H_1 and H_1' are obtained from the component F of $G_1 - v$, containing u_1, and G_2 by the same operation as G and G' are did from G_1 and G_2 described in the lemma. If F is the trivial graph, then $H_1' \cong G_2 \cong H_1$, and thus $a(H_1') \geq a(H_1)$; if F is nontrivial, by the induction hypothesis, we also have $a(H_1') \geq a(H_1)$. Hence $a(G' - v) \geq a(G - v)$. In addition, by Lemma 4.2, we know that $a(G - w)) > a(G_1) + a(G_2)$. Therefore,

$$\begin{aligned}
a(G') &= a(G' - u) + a(G' - w) + \sum_{v \in V(G)} a(G' - v) \\
&= a(G_1 - u_1) + a(G_2 - u_2) + a(G' - w) + \sum_{v \in V(G) \setminus \{u, w\}} a(G' - v) \\
&> a(G_1 - u_1) + a(G_2 - u_2) + a(G_1) + a(G_2) + \sum_{v \in V(G) \setminus \{u, w\}} a(G - v) \\
&= a(G - u_1) + a(G - u_2) + \sum_{v \in V(G) \setminus \{u_1, u_2\}} a(G - v) \\
&= a(G).
\end{aligned}$$

By the similar argument as above, one can prove that if $n_1 + n_2 \geq 5$, then $b(G') > b(G)$, too. Thus $b(G) = b(G')$ if and only if $G_1 \cong G_2 \cong K_2$. $\square$

Theorem 4.4. Let T be a tree of order $n \geq 4$. Then

(1) $2 \cdot 3^{n-3} \leq a(T) \leq (n-1)!(1 + \frac{1}{2!} + \frac{1}{3!} + \cdots + \frac{1}{(n-2)!})$, with the left-hand side of equality if and only if $T \cong P_n$, and with the right-hand side of equality if and only if $T \cong K_{1,n-1}$.

(2) $2 \cdot 3^{n-3} \leq b(T) \leq (n-1)!$, and for $n \geq 5$, $2 \cdot 3^{n-3} = b(T)$ if and only if $T \cong P_n$; $b(T) = (n-1)!$ if and only if $T \cong K_{1,n-1}$.

Proof. Let T be a tree of order n with maximum $a(T)$ (or respectively, $b(T)$) among all trees of order n. By contradiction, suppose $T \cong K_{1,n-1}$. Then it is clear that there exists an edge $e \in E(G)$ such that the two components of $T - e$, T_1 and T_2, say, are both nontrivial. Let u_i be the end vertex of e in T_i, and T' be the graph obtained from T_1 and T_2 by identifying u_1 and u_2 as vertex u, and adding a new vertex w and joining it to u. By Lemma 4.3, $a(T) < a(T')$ (or respectively, $b(T) < b(T')$), which contradicts with the choice of T. Thus T must be the star, and thus by Proposition 2.3, the right-hand sides of inequalities (1) and (2) hold, with the equalities if and only if $T \cong K_{1,n-1}$.

We prove the the left sides of the two inequalities by induction on the order of trees. Note that there are exactly two non-isomorphic trees of order 4, namely, P_4 and $K_{1,3}$. By Propositions 2.2 and 2.3, $b(P_4) = b(K_{1,3}) = 4$. Next suppose T is a tree of order $n \geq 5$ and is not the path

P_n. Then T has at least three vertices v_1, v_2 and v_3, say, of degree 1 and another vertices v_4, say, such that $T - v_4$ is not an empty graph. So $T - v_i$ is a tree of order $n - 1 \geq 4$, by induction hypothesis, $b(T - v_i) \geq b(P_{n-1})$, and by Corollary 3.2, $b(T - v_4) > 0$. This gives

$$b(T) = \sum_{v \in V(G)}^{n} b(T - v_i) = \sum_{i=1}^{4} b(T - v_i) > 3b(P_{n-1}) = b(P_n).$$

On the other hand,

$$a(T) = \sum_{v \in V(G)}^{n} a(T - v_i) \geq \sum_{i=1}^{3} a(T - v_i) > 3b(P_{n-1}) = b(P_n).$$

Combining with Proposition 2.2, we have $a(T) = 2 \cdot 3^{n-3}$ (or $b(T) = 2 \cdot 3^{n-3}$) if and only if $T \cong K_{1,n-1}$. □

It was pointed out in [5] that, for any tree T of order n, $a(T) > b(T)$ except for $T \cong P_n$ when $a(P_n) = b(P_n)$. Here we prove the statement.

Theorem 4.5. If T is a tree and $\mid V(T) \mid \geq 3$, then $a(T) \geq b(T)$, the equality holds if and only if T is a path.

Proof. We use induction on the order n of T. If $\mid V(T) \mid = 3, 4$ it is easy to see that the theorem is true. So we assume that $n > 4$ and the theorem holds for smaller values of n.

Let $V(T) = \{v_1, v_2, \cdots, v_n\}$, then the dissection of T is the sum of the dissection of all the components of $T - v_1, T - v_2, \cdots, T - v_n$. For any component T' of $T - v_1, T - v_2, \cdots, T - v_n$, if $\mid V(T') \mid \geq 3$, then by hypothesis $a(T') \geq b(T')$. If $\mid V(T') \mid = 2$, then T' is an edge. Let $V(T') = \{v_1, v_2\}$, T' a component of $T - v_i$. Without loss of generality, suppose v_1 is adjacent to v_i, then v_1 is of degree 2 and v_2 is of degree 1 in T. Hence v_2 is an isolated vertex in $T - v_1$, and so, in all the components of $T - v_1, \cdots, T - v_n$, the number of the isolated vertices is larger than or equal to the number of the edges. Now it follows that $a(T) \geq b(T)$. If T is not a path, then there is at least one component T_j of $T - v_i$ $(i = 1, 2, \cdots, n)$ having order $n - 1$ and being not a path. By the induction hypothesis $a(T_j) > b(T_j)$, and so $a(T) > b(T)$. The proof is complete. □

References

[1] J.A. Bondy, U.S.R. Murty, Graph Theory with Applications, Macmillan, London and Elsevier, New York, 1976.

[2] C. Hu and L. Xu, Developing molecullar identification numbers by an all-paths method, J. Chem. Inf. Comput. Sci. **37**(1997), 311-315.

[3] M. Randic, On dissection of acyclic graphs, MATCH Commun. Math. Comput. Chem. **5** (1979) 135-148.

[4] M. Randic, On molecular indentification numbers, J. Chem. Inf. Comput. Sci. **24** (1984) 164-175.

[5] M. Randic, X. Guo, and P. Calkins, Graph dissection revisited : Application to smaller Alikanes, Acta Chim. Slov., **47** (2000), 489-506.

[6] M. Randic and W.L. Woodworth, Characterization of acyclic graphs by successive dissection, MATCH Commun. Math. Comput. Chem. **13** (1982), 291-313.