

# CALCULATING THE DEGREE DISTANCE OF PARTIAL HAMMING GRAPHS

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## Abstract

If  $G$  is a connected graph with vertex set  $V(G)$ , then the degree distance of  $G$  is defined as  $DD(G) = \sum_{\{u,v\} \in V(G)} (\deg u + \deg v)d(u,v)$ , where  $\deg u$  is the degree of vertex  $u$ , and  $d(u,v)$  denotes the distance between  $u$  and  $v$ . In the chemical literature,  $DD(G)$  is better known under

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the name *Schultz index*. In the class of partial Hamming graphs, which include trees, benzenoid and phenylene systems among others, we express the degree distance in terms of the canonical metric representation, thus simplifying its computation.

## 1 Introduction

Let  $G$  be a connected graph of order  $n$  and  $V(G)$  its vertex set. We denote the degree of a vertex  $u \in V(G)$  by  $\deg u$  and the distance between vertices  $u$  and  $v \in V(G)$  by  $d(u, v)$ . The *degree distance* of  $G$  is defined as

$$DD(G) = \sum_{\{u,v\} \in V(G)} (\deg u + \deg v) d(u, v).$$

The degree distance seems to have been considered first in connection with certain chemical applications by Dobrynin and Kochetova [1] and at the same time by Gutman [2], who named it the *Schultz index*. This name was eventually accepted by most other authors (see, e.g., [3, 4, 5]). In fact, there are several names (degree distance, MTI index, Schultz index, Zagreb index) associated to this index or closely related indices, we refer to [6] for a clarification of these notions.

The degree distance may be considered a weighted version of the Wiener index [7, 8]. Recall that the Wiener index of  $G$  is defined as

$$W(G) = \sum_{\{u,v\} \in V} d(u, v).$$

The relations between the degree distance and the Wiener index were studied in [2, 3, 9, 10, 11, 12]. An example of such relation,

$$DD(T) = 4W(T) - n(n - 1),$$

which holds whenever  $T$  is a tree of order  $n$  may be found in [2, 11].

In the mathematical literature, extremal properties of  $DD(G)$  were investigated in [13, 14, 15, 16, 17]. For the recent results on the Schultz molecular topological index see [18, 19, 20].

Here we show that  $DD(G)$  can be expressed in terms of the quotient graphs of the canonical metric representation of  $G$ . The metrics of the quotient graphs can be omitted when  $G$  is isometrically embeddable into a Hamming graph, which significantly simplifies calculation of

the degree distance for partial Hamming graphs. A similar approach has been recently used to calculate the Wiener index of a graph via its canonical metric representation [21].

In the rest of this section we present necessary concepts, while in the next section the main result is proved and a few examples given. The third section further specializes into calculating degree distance of benzenoid systems.

The *Cartesian product*  $G_1 \square \cdots \square G_k$  of graphs  $G_1, \dots, G_k$  has the vertex set  $V(G_1) \times \cdots \times V(G_k)$ , two vertices  $(u_1, \dots, u_k)$  and  $(v_1, \dots, v_k)$  being adjacent if they differ in exactly one position, say in  $i$ th, and  $u_i v_i$  is an edge of  $G_i$ . Let  $d_G$  stands for the usual geodesic distance in  $G$ . It is well-known that for  $G = G_1 \square \cdots \square G_k$  and vertices  $u, v \in G$  we have  $d_G(u, v) = \sum_{i=1}^k d_{G_i}(u_i, v_i)$ , see [22].

A *Hamming graph* is the Cartesian product of complete graphs and a *partial Hamming graph* is a graph that isometrically (that is, distance preserving) embeds into a Hamming graph. In the particular case where all the factors are  $K_2$ 's we speak of *hypercubes* and *partial cubes*, respectively, whose important examples include trees, median graphs, benzenoids, phenylenes, grids, bipartite torus graphs, ... Partial Hamming graphs have been studied and characterized in [23, 24, 25].

The canonical metric representation of a connected graph  $G$ , due to Graham and Winkler [26], is defined as follows. Edges  $xy$  and  $uv$  of  $G$  are in the Djoković–Winkler [27, 28] relation  $\Theta$  if  $d(x, u) + d(y, v) \neq d(x, v) + d(y, u)$ . Let  $\Theta^*$  be the transitive closure of  $\Theta$  and let  $E_1, \dots, E_k$  be the  $\Theta^*$ -equivalence classes,  $\Theta^*$ -classes for short. For  $i = 1, \dots, k$ , let  $G_i$  denote the graph  $(V(G), E(G) \setminus E_i)$  and  $C_1^{(i)}, \dots, C_{r_i}^{(i)}$  the connected components of  $G_i$ . As an example, consider the graph  $G$  from Fig. 1. It has two  $\Theta^*$ -classes  $E_1$  and  $E_2$ . The graphs  $G_1$  and  $G_2$  are also shown.

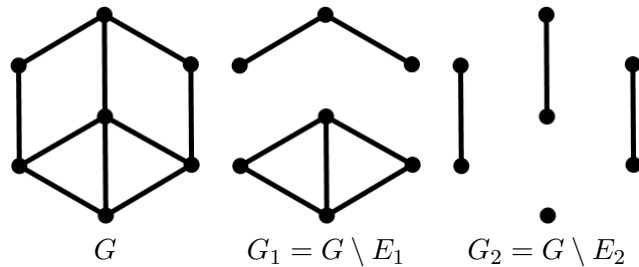


Figure 1:  $\Theta^*$ -equivalence classes of  $G$ .

Define the graphs  $G_i^*$ ,  $i = 1, \dots, k$ , with  $V(G_i^*) = \{C_1^{(i)}, \dots, C_{r_i}^{(i)}\}$  where  $C_j^{(i)}C_{j'}^{(i)}$  is an edge of  $G_i^*$  if some vertex of  $C_j^{(i)}$  is in  $G$  adjacent to a vertex of  $C_{j'}^{(i)}$ . Let the contractions  $\alpha_i: V(G) \rightarrow V(G_i^*)$  be given by  $\alpha_i(v) = C_j^{(i)}$  where  $v \in C_j^{(i)}$ . Then the mapping

$$\alpha: G \rightarrow G_1^* \square \dots \square G_k^*, \quad (1)$$

where  $\alpha(v) = (\alpha_1(v), \dots, \alpha_k(v))$ , is the *canonical metric representation* of the graph  $G$ . Graham and Winkler proved, among others, that  $\alpha$  is an irredundant isometric embedding. Here *irredundant* means that every factor graph  $G_i^*$  has at least two vertices and that each vertex of  $G_i^*$  appears as a coordinate of some vertex  $\alpha(u)$ . For more results on the canonical representation we refer to the papers [29, 30, 31] and the books [32, 22].

## 2 The main result

**Theorem 2.1** *Let  $G = (V, E)$  be a partial Hamming graph. Let the notations of its canonical metric representation be as in (1) and let  $d_i$  be the distance function of  $G_i^*$ . For  $i = 1, \dots, k$  and  $j = 1, \dots, r_i$ , let  $\deg C_j^{(i)}$  be the sum of degrees in  $G$  of vertices that are mapped to  $C_j^{(i)}$  by  $\alpha_i$ . Then*

$$DD(G) = \sum_{i=1}^k \sum_{j=1}^{r_i} \deg C_j^{(i)} (n - |C_j^{(i)}|).$$

**Proof.** Let  $\alpha: G \rightarrow G^* = G_1^* \square \dots \square G_k^*$  be the canonical representation of  $G$ , where for  $u \in V$ ,  $\alpha(u) = (\alpha_1(u), \dots, \alpha_k(u))$ . Then we can compute as follows:

$$\begin{aligned} DD(G) &= \sum_{\{u,v\} \in V} (\deg u + \deg v) d_G(u, v) = \sum_{\{u,v\} \in V} (\deg u + \deg v) d_{G^*}(\alpha(u), \alpha(v)) \\ &= \sum_{\{u,v\} \in V} (\deg u + \deg v) \sum_{i=1}^k d_i(\alpha_i(u), \alpha_i(v)) \\ &= \sum_{i=1}^k \sum_{\{u,v\} \in V} (\deg u + \deg v) d_i(\alpha_i(u), \alpha_i(v)). \end{aligned}$$

Since  $G$  is a partial Hamming graph, each  $G_i^*$  is a complete graph, so that  $d_i(\alpha_i(u), \alpha_i(v)) = 1$

whenever  $\alpha_i(u) \neq \alpha_i(v)$ . Thus,

$$\begin{aligned}
DD(G) &= \sum_{i=1}^k \sum_{\{u,v\} \in V, \alpha_i(u) \neq \alpha_i(v)} \deg u + \deg v \\
&= \sum_{i=1}^k \sum_{u \in V} \deg u (n - |\alpha_i(u)|) \\
&= \sum_{i=1}^k \sum_{j=1}^{r_i} \sum_{u \in \alpha_i^{-1}(C_j^{(i)})} \deg u (n - |C_j^{(i)}|) \\
&= \sum_{i=1}^k \sum_{j=1}^{r_i} \deg C_j^{(i)} (n - |C_j^{(i)}|).
\end{aligned}$$

□

In the case of partial cubes, Theorem 2.1 specializes to an even more applicable form. For this sake some preparation is needed. It is not difficult to observe that  $G$  is a partial cube if and only if every  $G_i^*$  of its canonical metric representation is isomorphic to  $K_2$ . Hence every corresponding graph  $G_i$  consists of two connected components, they are denoted  $W_{i,0}$  and  $W_{i,1}$  and called *halfspaces* of  $G$ . In other words,  $W_{i,\chi}$  consists of those vertices  $u$  of  $G$  for which  $\alpha_i(u) = \chi$ ,  $\chi \in \{0, 1\}$ .

Let  $G$  be a partial cube with halfspaces  $W_{i,\chi}$ ,  $1 \leq i \leq k$ ,  $\chi \in \{0, 1\}$ . For any  $1 \leq i \leq k$  and any  $\chi \in \{0, 1\}$  we set

$$D_{(i,\chi)} = \sum_{u \in W_{(i,\chi)}} \deg(u).$$

Since  $r_i = 2$  for any  $i$  and  $|W_{(i,\chi)}| + |W_{(i,\bar{\chi})}| = n$ , Theorem 2.1 reduces to:

**Corollary 2.2** *Let  $G$  be a partial cube with halfspaces  $W_{i,\chi}$ ,  $1 \leq i \leq k$ ,  $\chi \in \{0, 1\}$ . Then*

$$DD(G) = \sum_{i=1}^k (|W_{(i,0)}| D_{(i,1)} + |W_{(i,1)}| D_{(i,0)}).$$

An advantage of Corollary 2.2 comparing to computing  $DD(G)$  by the definition is that we need not to compute distance but only count vertices and sum up the degrees. This result can be considered as another instance of the so-called cut method. For its general description and an overview of its applications in chemical graph theory see [33]. The method got its name because of benzenoid graph in which the  $\Theta^*$ -classes are precisely the orthogonal cuts. We also mention

a related result on the Wiener index of weighted graphs from [34]. In that case, however, the weighted Wiener index was defined as  $\sum_{u,v} w(u)w(v)d(u,v)$ , where  $w$  is an arbitrary weight function.

### 3 Applications to chemical graphs

In this section we will apply Corollary 2.2 to a particular, but chemically very important class of partial cubes—benzenoid graphs.

The term *benzenoid graph* is used for graphs constructed in the following manner. Consider the hexagonal lattice  $\mathcal{H}$ . Let  $Z$  be a circuit on this lattice. Then benzenoid graphs are formed by the vertices and edges of  $\mathcal{H}$  lying on some circuit  $Z$  or in its interior. The vertices and edges belonging to  $Z$  form the perimeter of the respective benzenoid graph, while the vertices (if any) not belonging to the perimeter are said to be the internal vertices.

We first present two simple classes of chemical graphs to get the idea how Corollary 2.2 is used.

#### 3.1 Linear benzenoid chains

Consider the linear benzenoid chain  $L_h$ , see Fig. 3.1 for its description.

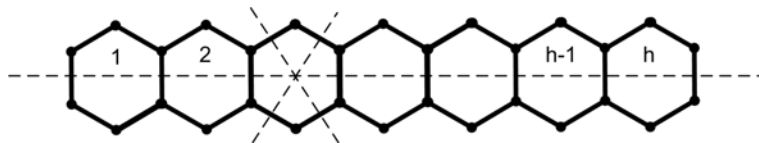


Figure 2: The linear benzenoid chain  $L_h$

The number of vertices equals  $n_h = 4h + 2$ , while the sum of all degrees equals  $d_h = 2m_h = 10h + 2$  since there are  $2(h - 1)$  vertices of degree three and  $(2h + 4)$  vertices of degree two. For the horizontal orthogonal cut we have the contribution  $2(2h + 1)(5h + 1)$ . For the hexagon  $C_i$ , there are two symmetrical orthogonal cuts with contributions

$$(n_{i-1} + 1) \cdot (d_{n-i} + 4) + (n_{h-i} + 1) \cdot (d_i + 4).$$

Using again the symmetry, one has

$$\begin{aligned}
 DD(L_h) &= 2(2h+1)(5h+1) + 4 \sum_{i=1}^k (4(i-1)+3)(10(h-i)+6) \\
 &= 2 \left( 10h^2 + 7h + 1 + 2 \sum_{i=1}^k (40ih - 10h - 40i^2 + 34i - 6) \right) \\
 &= \frac{2}{3} (40h^3 + 72h^2 + 47h + 3).
 \end{aligned}$$

### 3.2 Linear phenylenes

Consider the linear phenylene  $PH_h$ , consisting of  $h-1$  four-membered (cyclobutadiene) and  $h$  six-membered (benzene) rings, in which each cyclobutadiene unit is adjacent to two benzene rings, whereas benzene rings are not adjacent to each other, see Fig. 3.2.

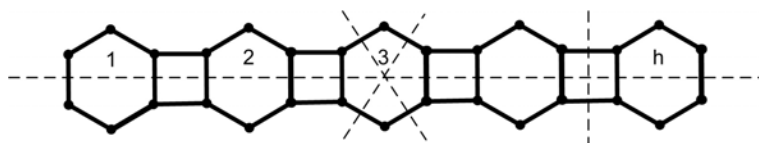


Figure 3: The linear phenylene  $PH_h$

The number of vertices equals  $n_h = 6h$ , while the sum of all degrees equals  $d_h = 2m_h = 2(8h-2)$ . The horizontal cut of  $PH_h$  contains  $2h$  edges, while any of the remaining  $(h-1)+2h$  cuts contains two edges. For the horizontal orthogonal cut we have the contribution  $2 \cdot 3h(8h-2)$ . For vertical cut at cyclobutadiene  $i$ , we have contribution  $6i(16(h-i)-2) + 6(h-i)(16i-2)$ , and for the hexagon  $C_i$ , there are two symmetrical orthogonal cuts with contributions  $(6i-3)(16(h-i)+6) + (6(h-i)+3)(16i-10)$ . Therefore,

$$DD(PH_h) = 12h^2(8h+1).$$

### 3.3 Coronene/circumcoronene series

We next obtain a closed expression for the degree distance of the coronene/circumcoronene homologous series  $H_k$ ,  $k \geq 1$ . The first terms of this series are  $H_1 = \text{benzene}$ ,  $H_2 = \text{coronene}$ ,  $H_3 = \text{circumcoronene}$ ,  $H_4 = \text{circumcircumcoronene}$ , see Fig. 3.3 where  $H_3$  is shown.

In Fig. 3.3,  $2k-1$  horizontal elementary cuts of  $H_k$  are indicated. There exist two additional groups of  $2k-1$  equivalent cuts, obtained by rotating the former group by  $+60^\circ$  and  $-60^\circ$ . The

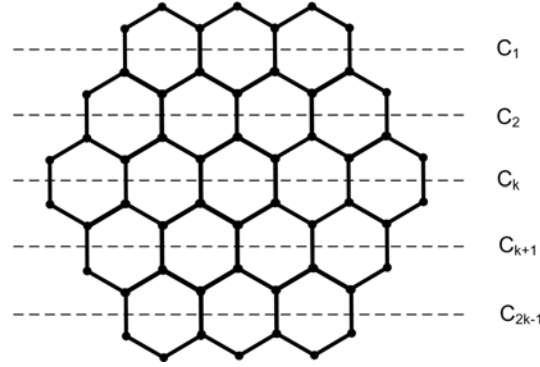


Figure 4: The Coronene / Circumcoronene  $H_3$ .

number of vertices of  $H_k$  equals  $n_k = 6k^2$ , while there are exactly  $6k$  vertices of degree two. Therefore, the sum of all degrees equals

$$d_k = 2m_k = 2 \cdot 6k + 3 \cdot (6k^2 - 6k) = 6k(3k - 1).$$

It should be observed that because of symmetry, the contribution of the elementary cut  $C_i$  is equal to the contribution of  $C_{2k-i}$ ,  $i = 1, 2, \dots, k - 1$ . It can be shown by induction that for  $i = 1, 2, \dots, k$  the number of vertices above cut  $C_i$  equals  $i(2k + i)$ , while the sum of degrees of the vertices is  $(6k - 1)i - 2i + 3i^2$ . Therefore,

$$\begin{aligned} \frac{1}{3}DD(H_k) &= 2 \cdot (3k^2)(9k^2 - 3k) \\ &+ 2 \sum_{i=1}^{k-1} i(2k + i) \cdot (18k^2 - 6k - ((6i - 1)k - 2i + 3i^2)) \\ &+ 2 \sum_{i=1}^{k-1} (6k^2 - i(2k + i)) \cdot ((6i - 1)k - 2i + 3i^2) \\ &= \frac{2h}{15} \cdot (3 + 25h - 45h^2 - 205h^3 + 492h^4). \end{aligned}$$

Finally, we derive the fifth-order polynomial formula for the degree distance of  $H_k$ .

$$DD(H_k) = \frac{2}{5} \cdot h (3 + 25h - 45h^2 - 205h^3 + 492h^4).$$

## 4 Linear algorithm for benzenoid systems

Let  $B$  be a benzenoid graph. The edge set of  $B$  can be partitioned into three cuts as follows: each cut consists of all parallel edges. Then, making quotient graphs just as it is done in the canonical

metric representation, we obtain three trees  $T_1, T_2, T_3$ . The key observation of Chepoi [35] is that  $B$  embeds isometrically into  $T_1 \square T_2 \square T_3$  (see [36, 37, 38, 39] for algorithms for calculating Wiener index, Szeged index and hyper-Wiener index in benzenoid systems and trees).

Let

$$W(T, a, b) = \sum_{v \in T} \sum_{u \in T} (a(u)b(v) + a(v)b(u))d(u, v)$$

be the modified weighted Wiener index of tree  $T$ , such that every vertex  $v \in T$  has two weight values  $a(v)$  and  $b(v)$ .

For  $i = 1, 2, 3$ , define the weight  $a_i$  to be the number of vertices and  $b_i$  to be the sum of degrees in the corresponding connected component.

**Theorem 4.1** *Let  $G$  be a benzenoid system and let  $\alpha$  be the canonical embedding of  $G$  into  $H = T_1 \square T_2 \square T_3$ . Then*

$$DD(G) = W(T_1, a_1, b_1) + W(T_2, a_2, b_2) + W(T_3, a_3, b_3).$$

**Proof.** For  $u \in V$ , let  $\alpha(v) = (v_1, v_2, v_3)$ .

$$\begin{aligned} DD(G) &= \sum_{v \in V} \sum_{u \in V} (deg(v) + deg(u)) \cdot d(u, v) \\ &= \sum_{v \in V} \sum_{u \in V} (deg(v) + deg(u)) \cdot d_H(\alpha(u), \alpha(v)) \\ &= \sum_{v \in V} \sum_{u \in V} (deg(v) + deg(u)) \cdot \sum_{i=1}^3 d_{T_i}(u_i, v_i) \\ &= \sum_{i=1}^3 \left( \sum_{v \in V} \sum_{u \in V} (deg(v) + deg(u)) \cdot d_{T_i}(u_i, v_i) \right) \\ &= \sum_{i=1}^3 \left( \sum_{v_i \in V(T_i)} \sum_{u_i \in V(T_i)} (b_i(v) a_i(u) + b_i(u) a_i(v)) \cdot d_{T_i}(u_i, v_i) \right) \\ &= W(T_1, a_1, b_1) + W(T_2, a_2, b_2) + W(T_3, a_3, b_3). \end{aligned}$$

Let us take a closer look at the identity

$$\sum_{v \in V} \sum_{u \in V} (deg(v) + deg(u)) \cdot d_{T_i}(u_i, v_i) = \sum_{v_i \in V(T_i)} \sum_{u_i \in V(T_i)} (b_i(v) a_i(u) + b_i(u) a_i(v)) \cdot d_{T_i}(u_i, v_i).$$

Consider two vertices  $v_k$  and  $u_k$  from  $T_k$ ,  $k = 1, 2, 3$ , and assume that they represent components consisting of vertices  $v'_1, v'_2, \dots, v'_p$  and  $u'_1, u'_2, \dots, u'_q$  from  $T$ , respectively.

$$\begin{aligned}
S &= \sum_{i=1}^p \sum_{j=1}^q (deg(v'_i) + deg(u'_j)) \cdot d_{T_k}(v_k, u_k) \\
&= d_{T_k}(v_k, u_k) \cdot \left( p \sum_{j=1}^q deg(u'_j) + q \sum_{i=1}^p deg(v'_i) \right) \\
&= d_{T_k}(v_k, u_k) \cdot (a_k(v)b_k(u) + a_k(u)b_k(v)).
\end{aligned}$$

□

We will present the linear algorithm for calculating the following generalization of weighted Wiener index.

**Lemma 4.2** *Let  $(T, a, b)$  be a double vertex-weighted tree. For an edge  $e$  of  $T$ , denote with  $T_1$  and  $T_2$  the connected components of  $T \setminus e$  and for  $i = 1, 2$  set*

$$A_i(e) = \sum_{u \in T_i} a(u) \quad \text{and} \quad B_i(e) = \sum_{u \in T_i} b(u).$$

Then we have

$$W(T, a, b) = \sum_{e \in T} (A_1(e)B_2(e) + A_2(e)B_1(e)).$$

Using the fact that  $A_1(e) + A_2(e) = \sum_{v \in T} a(v) = A$  and  $B_1(e) + B_2(e) = \sum_{v \in T} b(v) = B$ , one can easily extend the dynamic algorithm for calculating the sums  $A_1(e)$  and  $B_1(e)$  in tree  $T$ . Choose an arbitrary vertex  $v$  as the root and perform depth-first search from  $v$ . Denote with  $p(v)$  the parent of vertex  $v$  in the DFS tree. Let  $A(v)$  denote the sum of vertex weights  $a$  in the subtree rooted at  $v$  (including  $a(v)$ ), while  $B(v)$  denotes the sum of vertex weights  $b$  in the subtree rooted at  $v$  (including  $b(v)$ ). Using the formulas

$$A(v) = a(v) + \sum_{(u,v) \in E(T)} A(u) \quad \text{and} \quad B(v) = b(v) + \sum_{(u,v) \in E(T)} B(u),$$

one can easily calculate the arrays  $A$  and  $B$ , while traversing vertices in the recursive call of depth-first search. Finally notice that  $A_1((v, p(v))) = A(v)$  and  $B_1((v, p(v))) = B(v)$ .

The time complexity of the algorithm for calculating the modified weighted Wiener index is  $O(n)$ , and the memory used is  $O(n)$ , since we need three additional arrays of length  $n$ .

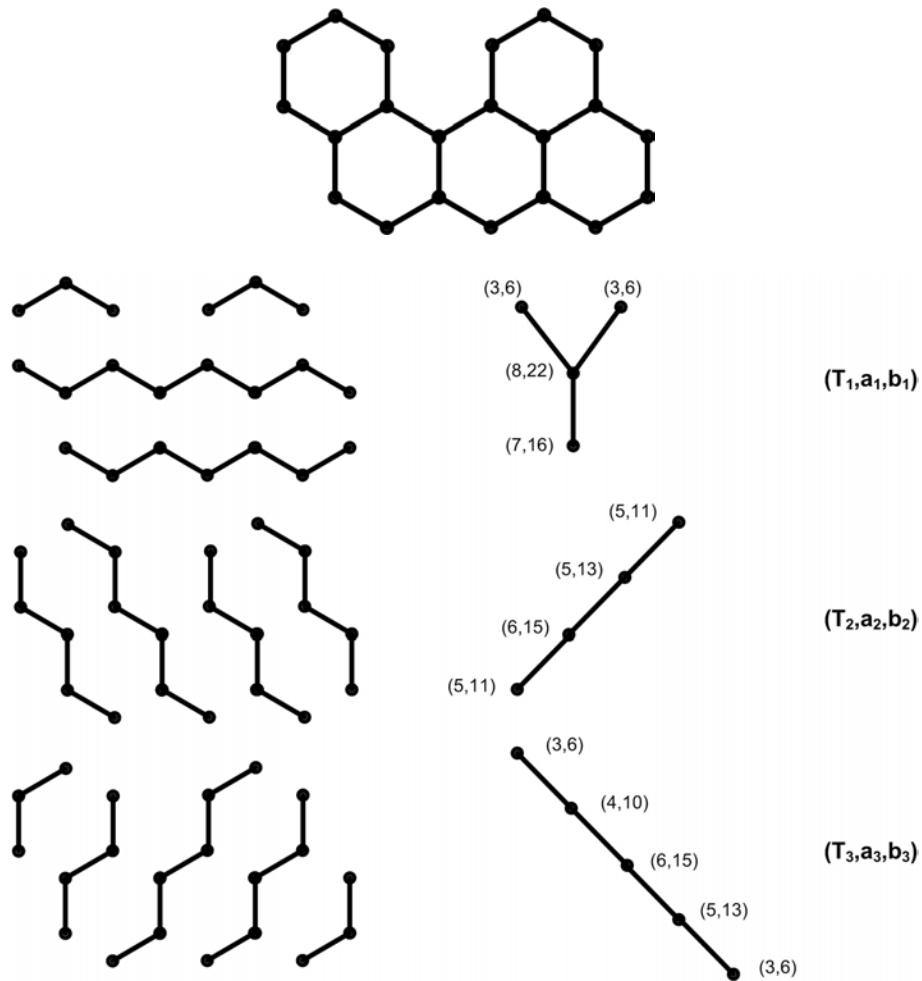


Figure 5: Steps in computing  $DD$  of the benzenoid system  $G$

$$DD(T_1, a_1, b_1) = (3 \cdot 44 + 18 \cdot 6) + (7 \cdot 34 + 16 \cdot 14) + (18 \cdot 6 + 3 \cdot 44) = 942$$

$$DD(T_2, a_2, b_2) = (5 \cdot 39 + 16 \cdot 11) + (10 \cdot 26 + 11 \cdot 24) + (16 \cdot 11 + 5 \cdot 39) = 1266$$

$$DD(T_3, a_3, b_3) = (3 \cdot 44 + 18 \cdot 6) + (7 \cdot 34 + 14 \cdot 16) + (13 \cdot 19 + 8 \cdot 31) + (18 \cdot 6 + 3 \cdot 44) = 1437$$

By Theorem 4.1, we have  $DD(G) = 942 + 1266 + 1437 = 3645$ .

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