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# THE LATTICE DIMENSION OF BENZENOID SYSTEMS

**Sandi Klavžar**[a,b,*] and **Matjaž Kovše**[b]

[a]Department of Mathematics and Computer Science
PeF, University of Maribor
Koroška cesta 160, SI–2000 Maribor, Slovenia
sandi.klavzar@uni-mb.si

[b]Institute of Mathematics, Physics and Mechanics
Jadranska 19, 1000 Ljubljana, Slovenia
matjaz.kovse@guest.arnes.si

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**Abstract**

A labeling of vertices of a benzenoid system $B$ is proposed that reflects the graph distance in $B$ and is significantly shorter than the labeling obtained from a hypercube embedding of $B$. The new labeling corresponds to an embedding of $B$ into the integer lattice $\mathbb{Z}^d$ and is shown to be optimal for all practical purposes. A coordinatization algorithm is presented and it is demonstrated that it can be easily carried out by hand.

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# 1 Introduction

Benzenoid systems (molecular graphs of benzenoid hydrocarbons) are one of the most studied classes of graphs within the chemical graph theory, we refer to the books [6, 12] dedicated to these systems and a sample of papers on different aspects of these graphs [7, 9, 10, 14, 21–29]. It is therefore not surprising that many names have been given to benzenoid systems, notably hexagonal systems. (For the list of all names see [10].)

One of the important features of benzenoid systems is that they can be isometrically embedded into hypercubes, the fact first observed in [18]. This observation led to many investigations of benzenoid systems [2, 4, 5, 15, 19], to investigations of other chemical graphs that can also be isometrically embedded into hypercubes, for instance of phenylenes, see [13], and to more general embeddings of (chemical) graphs [3].

It clearly turned out that an isometric embedding of a benzenoid system into a hypercube has many advantages. There is, however, one drawback of this approach. The number of coordinates of an embedding of a benzenoid system $B$ into a hypercube is equal to the number of the elementary cuts of $B$. Therefore, if $B$ is not very small, the vertex labels become large. Hence for bigger benzenoid systems the investigations are not easily carried out "by hand". In this paper we propose another labeling of benzenoid systems that also reflects the vertex distance but is significantly shorter than the labeling obtained from the isometric hypercube embedding. To be more precise, we label vertices $u$ of a benzenoid system $B$ with labels

$$\ell(u) = (\ell_1(u), \ell_2(u), \ldots, \ell_d(u)), \quad \ell_1(u), \ldots, \ell_d(u) \in \mathbb{Z},$$

such that

$$d_B(u,v) = \sum_{i=1}^{d} |\ell_i(u) - \ell_i(v)|,$$

where $d_B(u,v)$ is the usual shortest path distance in $B$. Such embeddings of graphs into $\mathbb{Z}^d$ are called *lattice embeddings*. The minimum possible $d$ for which there exists a lattice embedding of $B$ is called the *lattice dimension* of $B$ and denoted $\dim_L(B)$. It is well known, cf. [11], that a graph $G$ has a lattice embedding if and only if $G$ is an isometric subgraph of a hypercube. As the latter is true for benzenoid systems [18], the lattice dimension is well-defined for them.

The paper is organized as follows. In the next section we introduce the concepts needed in this paper, in particular, we define benzenoid systems, present their fundamental trees, and recall the 3-trees embedding from [2]. Then, in Section 3, we give a lower and an upper bound for the lattice dimension of a benzenoid system $B$. The two bounds are expressed in the number of leaves of the fundamental trees of $B$ and coincide in one half of the cases, while in the other cases they differ by 1. Hence for all practical purposes the proposed labelings are optimal. In Section 4 the labeling algorithm is described. We conclude with an example of such a labeling and with some remarks.

## 2 Preliminaries

*Benzenoid systems* are graphs constructed as follows [12]. Let $Z$ be a circuit on the benzenoid (graphite) lattice. Then a benzenoid system is formed by the vertices and edges of the lattice lying on $Z$ and in the interior of $Z$. Let $e$ be an edge of a benzenoid system $B$ lying on its perimeter $Z$. Then the *elementary cut* $C_e$ corresponding to $e$ is the set of all edges of $B$ such that with every edge $f \in C_e$, also the opposite edge with respect to a hexagon containing $f$ belongs to $C_e$. Note that the set of elementary cuts partitions the edge set of $B$.

Let $B$ be a benzenoid system. Then its edges can be naturally partitioned into three sets $E_1$, $E_2$, and $E_3$ consisting of (geometrically) parallel edges. In other words, $E_i$ is the union of elementary cuts in the same direction. For $i = 1,2,3$ let $B_i$ be the graph obtained from $B$ by removing all the edges of $E_i$. Let $T_i$ be the graph whose vertices are the connected components of $B_i$ (note that these components are paths), two such components $P'$ and $P''$ being adjacent in $T_i$ if there are vertices $u \in P'$ and $v \in P''$ such that $uv \in E_i$. Every $T_i$ is a tree, see [2, 4]. We call the trees $T_1$, $T_2$, and $T_3$ the *fundamental trees* of the benzenoid system $B$. An example of a benzenoid system $B$, the graphs $B_i$, and the fundamental trees of $B$ are shown in Figure 1. Chepoi [2] introduced fundamental trees and used them to calculate the diameter of benzenoids system. Later Chepoi and Klavžar [4] followed with a linear time algorithm for computation of the Wiener index.

A graph $H$ is an isometric subgraph of $G$ if $d_H(u,v) = d_G(u,v)$ for any vertices $u, v \in H$. In addition, a graph $H$ *isometrically embeds* into a graph $G$ if $H$ is isomorphic to an isometric subgraph of $G$.

The *Cartesian product* $G \,\square\, H$ of graphs $G$ and $H$ is the graph with vertex set $V(G) \times V(H)$ and $(a,x)(b,y) \in E(G \,\square\, H)$ whenever either $ab \in E(G)$ and $x = y$, or $a = b$ and $xy \in E(H)$.

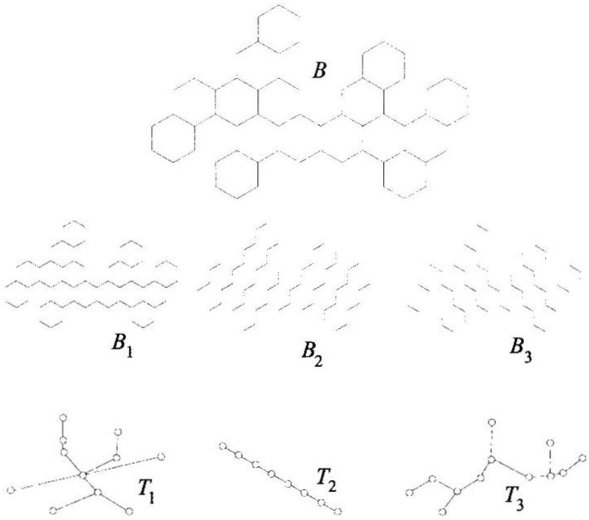


Figure 1: A benzenoid system $B$, the graphs $B_1$, $B_2$, $B_3$, and the fundamental trees $T_1$, $T_2$, $T_3$

The Cartesian product is associative, hence the product of several factors is well-defined. In particular, the Cartesian product $T_1 \square T_2 \square T_3$ has ordered triples $(u_1, u_2, u_3)$, $u_i \in T_i$, as vertices, and two such triples $(u_1, u_2, u_3)$ and $(v_1, v_2, v_3)$ are adjacent if and only if for some $i$, $u_i v_i \in E(T_i)$, and $u_j = v_j$ for $j \neq i$.

With these definitions we can now formulate the following result that is essential for our investigations.

**Theorem 2.1** (Chepoi [2]) *Let $B$ be a benzenoid system and $T_1, T_2, T_3$ its fundamental trees. Then $B$ isometrically embeds into the Cartesian product $T_1 \square T_2 \square T_3$.*

We recall that the distance function is additive on Cartesian products of graphs, see [17]. More precisely, let $G$ and $H$ be arbitrary graphs, and $(g, h), (g', h')$ vertices of $G \square H$. Then

$$d_{G \square H}((g,h),(g',h')) = d_G(g,g') + d_H(h,h') \, . \tag{1}$$

Finally, recall that a set of pairwise nonadjacent edges of a graph $G$ is called a *matching* of $G$.

# 3 Lattice dimension of benzenoid systems

The infinite benzenoid lattice (also known as the mosaic $(6^3)$) can be embedded into cubical lattice $\mathbb{Z}^3$, see [8]. Therefore, every benzenoid system which is an isometric subgraph of the infinite benzenoid lattice embeds into $\mathbb{Z}^3$ and has lattice dimension 3. An example of a benzenoid system $B$ that embeds isometrically into $\mathbb{Z}^3$ is shown in Figure 2.

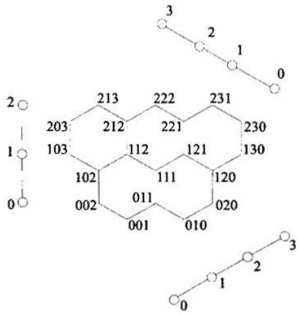


Figure 2: Example of benzenoid system which embeds isometrically into $\mathbb{Z}^3$

However, as soon as $B$ is not an isometric subgraph of the infinite benzenoid lattice, $\dim_{\mathrm{L}}(B) > 3$. In order to determine the lattice dimension of such benzenoid systems we will use a recent result of Eppstein from [11]. To describe it, the following concepts are needed.

For an edge $e = uv$ of $B$ let $W_{uv}$ and $W_{vu}$ be the connected components of $B \setminus C_e$, where $u \in W_{uv}$ and $v \in W_{vu}$. These subgraphs are called *semicubes* of $B$. The *semicube graph* $\mathrm{Sc}(B)$ of $B$ is the graph whose vertices are all the semicubes of $B$, two semicubes $W_{uv}$ and $W_{xy}$ being adjacent if $W_{uv} \cup W_{xy} = B$ and $W_{uv} \cap W_{xy} \neq \emptyset$.

Let $B$ be a benzenoid system. Then its *isometric dimension* $\dim_{\mathrm{I}}(B)$ is the number of elementary cuts of $B$. In other words, $\dim_{\mathrm{I}}(B) = |\mathrm{Sc}(B)|/2$.

Then Eppstein [11] proved (in a more general setting) the following theorem.

**Theorem 3.1** [11] *Let $B$ be a benzenoid system. Then*

$$\dim_{\mathrm{L}}(B) = \dim_{\mathrm{I}}(B) - |M|,$$

*where $M$ is any maximum matching in* $\mathrm{Sc}(B)$.

For our main theorem we need the following three lemmata. A proof of the second one can be found in [1, Lemma 2.3], while the last result has been independently discovered several times, probably for the first time in [16], see also [20].

**Lemma 3.2** *Let $B$ be a benzenoid system and $W_{uv}$ a semicube of $B$. Then $W_{uv}$ is an isolated vertex of* $\mathrm{Sc}(B)$ *if and only if $W_{uv}$ is a leaf of a fundamental tree of $B$.*

**Proof.** We observe first that $W_{uv}$ is an isolated vertex of $\mathrm{Sc}(B)$ if and only if no elementary cut of $B$ is completely contained in $W_{uv}$. Consequently, $W_{uv}$ is an isolated vertex of $\mathrm{Sc}(B)$ if and only if $W_{uv}$ is a path that lies on the perimeter of $B$. But this is equivalent to the fact that $W_{uv}$ is a leaf of the fundamental tree of $B$ that corresponds to the direction of $uv$. □

**Lemma 3.3** *Let $G$ and $H$ be isometric subgraphs of hypercubes. Then* $\dim_{\mathrm{L}}(G \,\Box\, H) = \dim_{\mathrm{L}}(G) + \dim_{\mathrm{L}}(H)$.

Since the Cartesian product is associative, Lemma 3.3 holds for any finite number of factors.

**Lemma 3.4** *Let $T$ be a tree. Then* $\dim_{\mathrm{L}}(T) = \lceil t/2 \rceil$, *where $t$ is the number of leaves of $T$.*

Now everything is ready for the next theorem.

**Theorem 3.5** *Let $B$ be a benzenoid system and let $t_i$ be the number of leaves of the fundamental tree $T_i$, $1 \le i \le 3$. Then*

$$\left\lceil \frac{t_1}{2} + \frac{t_2}{2} + \frac{t_3}{2} \right\rceil \le \dim_{\mathrm{L}}(B) \le \left\lceil \frac{t_1}{2} \right\rceil + \left\lceil \frac{t_2}{2} \right\rceil + \left\lceil \frac{t_3}{2} \right\rceil .$$

**Proof.** By Theorem 3.1, $\dim_{\mathrm{L}}(B) = \dim_{\mathrm{I}}(B) - |M|$, where $M$ is any maximum matching in $\mathrm{Sc}(B)$. Let $r$ be the number of isolated vertices of $\mathrm{Sc}(B)$. Then

$$|M| \le (|\mathrm{Sc}(B)| - r)/2$$

and by Lemma 3.2 we infer that

$$|M| \le (|\mathrm{Sc}(B)| - (t_1 + t_2 + t_3))/2 .$$

Therefore,

$$\begin{aligned}\dim_{\mathrm{L}}(B) &= \dim_{\mathrm{I}}(B) - |M| = |\mathrm{Sc}(B)|/2 - |M| \\ &\geq |\mathrm{Sc}(B)|/2 - ((|\mathrm{Sc}(B)| - (t_1 + t_2 + t_3))/2) \\ &= (t_1 + t_2 + t_3)/2\,,\end{aligned}$$

and since the lattice dimension is an integer, the lower bound is proved.

Let $B$ be isometrically embedded into the Cartesian product $T_1 \square T_2 \square T_3$ of its fundamental trees. Since $B$ is an isometric subgraph we infer that $\dim_{\mathrm{L}}(B) \leq \dim_{\mathrm{L}}(T_1 \square T_2 \square T_3)$. Therefore, Lemma 3.3 implies that

$$\dim_{\mathrm{L}}(B) \leq \dim_{\mathrm{L}}(T_1 \square T_2 \square T_3) = \dim_{\mathrm{L}}(T_1) + \dim_{\mathrm{L}}(T_2) + \dim_{\mathrm{L}}(T_3)\,.$$

Lemma 3.4 completes the proof. □

Note that Theorem 3.5 gives the exact lattice dimension of $B$ if at least two of $t_1$, $t_2$, and $t_3$ are even. If at least two of these integers are odd, the theorem approximates the dimension up to 1. So for practical (chemical) purposes the result is completely satisfactory. We do, however, conjecture, that the lower bound is actually always the exact dimension. (See the last example in the final section.) In what follows we use the embedding of a benzenoid system into the Cartesian product of its fundamental trees to obtain lattice coordinates. Thus we always attain the upper bound from Theorem 3.5.

# 4 Labelling algorithm

Let $B$ be a benzenoid system. As before, let $t_i$, $1 \leq i \leq 3$, be the number of leaves of the fundamental tree $T_i$ of $B$. In this section we present a simple procedure how to assigns labels of length

$$r = \left\lceil \frac{t_1}{2} \right\rceil + \left\lceil \frac{t_2}{2} \right\rceil + \left\lceil \frac{t_3}{2} \right\rceil$$

to the vertices of $B$ such that the labeling is a lattice embedding of $B$ into $\mathbb{Z}^r$.

The algorithm first determines the fundamental trees $T_1$, $T_2$, and $T_3$ as described in Section 2. Then, the labeling of $B$ is obtained by simply concatenating the corresponding labelings of the fundamental trees. Hence, it remains to describe an algorithm that labels trees. We review in a simple way the labeling algorithm from [16]. For this some preparation is needed.

Let $T$ be a tree. For vertices $u$ and $v$ of $T$ we denote by $P(u,v)$ the (unique) $u,v$-path. The *inner degree* of a path of $T$ is defined as $\Sigma_v(\deg(v)-2)$, where the summation runs over the inner vertices of $P$. Let $T'$ a subtree of $T$. For a vertex $u \in T \setminus T'$ we define the *$u,T'$-path* as the path between $u$ and the closest vertex to $u$ that lies in $T'$.

Let $T$ be a tree with $k$ leaves. We will write $\ell(v) = \ell_1(v)\ell_2(v)\ldots\ell_{\lceil k/2\rceil}(v)$ to denote the label of a vertex $v$ and $\mathbf{e}_i$ for the $i$-th unit vector (of length $\lceil k/2\rceil$). Now the labeling algorithm can be described as follows.

**Algorithm A (Lattice Coordinates of a Tree)**

Input: Tree $T$ with $k$ leaves.

Output: Lattice coordinates of vertices of $T$ of length $\lceil k/2\rceil$.

0. Set $T'$ be the empty graph.
1. Find leaves $u$ and $v$ of $T$ such that the inner degree of $P(u,v)$ is maximum.
2. For $x \in P(u,v)$ set $\ell(x) = t0\ldots0$, where $t = d(u,x)$.
3. $T' \leftarrow T' \cup P(u,v)$; $i \leftarrow 2$.
4. While $T' \neq T$ do
   - 4.1. Find leaves $u$ and $v$ of $T$, $u,v \in T \setminus T'$, such that the inner degrees of the $u,T'$-path $P(u,y)$ and the $v,T'$-path $P(v,z)$ are two largest ones.
   - 4.2. For $x \in P(u,y)$ set $\ell(x) = \ell(y) + t\,\mathbf{e}_i$, where $t = d(x,y)$.
   - 4.3. For $x \in P(v,z)$ set $\ell(x) = \ell(z) - t\,\mathbf{e}_i$, where $t = d(x,z)$.
   - 4.4. $T' \leftarrow T' \cup P(u,y) \cup P(v,z)$; $i \leftarrow i+1$.

The coordinatization algorithm needs some comments.

- Note that the vertices $y$ and $z$ from Step 4.1 may coincide.
- If $k$ is odd, then in the last step of the algorithm there is only one leaf left. In this case the path $P(v,z)$ is empty and nothing is done in Step 4.3.
- If we wish to have nonnegative coordinates only, we add to the $i$th coordinates of labels $-(\min_{v\in T}\ell_i(v))$. We will do so in our example.

To get lattice coordinates of some vertex $u$ of a benzenoid system simply concatenate labels $u_1$, $u_2$ and $u_3$ according to which component of $B_i$ vertex $u$ belongs. That this algorithm indeed

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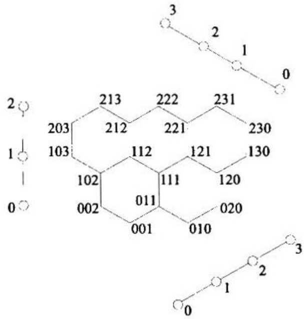


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The lattice embeddings of all three fundamental trees are presented in Figure 4, where also the final result is shown – the lattice embedding of $B$. In the figure the boldface label **4114310** of a vertex from $B$ is obtained by concatenation of the boldface labels **411**, **4**, and **310** from the corresponding fundamental trees.

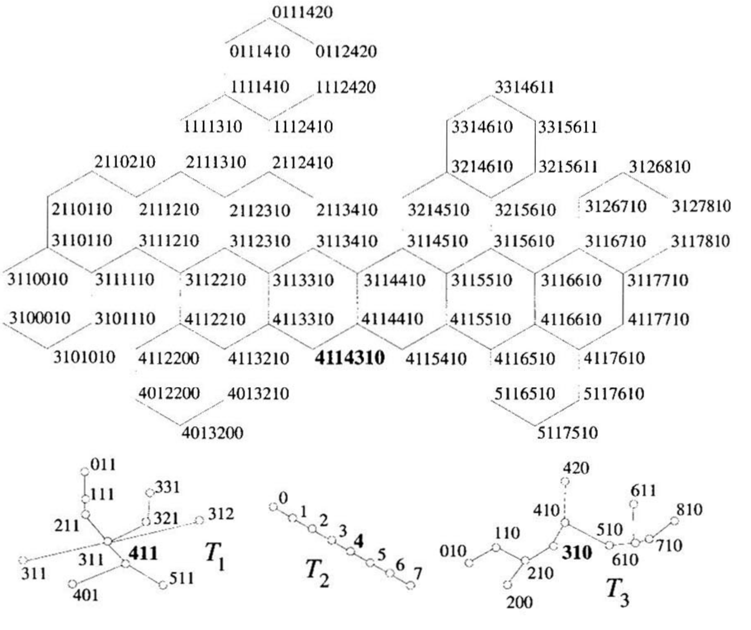


Figure 4: Lattice embedding of $B$.

We next give the smallest benzenoid system $B$ with the lattice dimension smaller than the dimension found by our algorithm. The system $B$ is shown in Figure 5. Since $\lceil 3/2 \rceil + \lceil 2/2 \rceil + \lceil 3/2 \rceil = 5$, our algorithm finds an embedding into $\mathbb{Z}^5$. On the other hand, $\dim_L(B) = 4$. To see this observe first that for the semicubes $W_{uv}$ and $W_{xy}$ of $\mathrm{Sc}(B)$ (see Figure 5) we have $W_{uv} \cup W_{xy} = B$ and $W_{uv} \cap W_{xy} \neq \emptyset$. Hence they are adjacent in the semicube graph $\mathrm{Sc}(B)$. Moreover, there exists a maximum matching in $\mathrm{Sc}(B)$ including the edge $W_{uv}W_{xy}$ and the remaining edges obtained by embedding trees $T_1 \setminus W_{vu}$ and $T_3 \setminus W_{yx}$ into $\mathbb{Z}$.

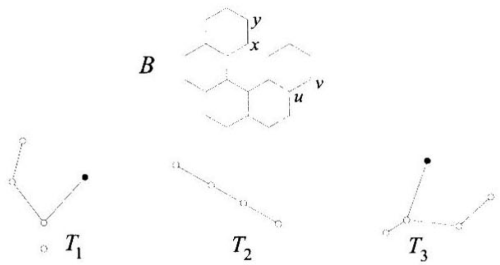


Figure 5: Semicubes $W_{vu}$ and $W_{yx}$ of Sc($B$) correspond to the leaves of the fundamental trees $T_1$ and $T_3$ that are colored black.

Similarly we can lower the dimension for one if at least two fundamental trees have an odd number of leaves, where each of the trees has a leaf with the neighbor of degree at least three.

As already mentioned, we conjecture that the lower bound from Theorem 3.5 is actually always the exact dimension. Another natural strengthening of presented results would be to find faster algorithm for lattice embeddings of trees.

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