DIMACS Series in Discrete Mathematics
and Theoretical Computer Science

Applications of Isometric Embeddings to Chemical Graphs

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ABSTRACT. Applications of isometric embeddings of benzenoid graphs are surveyed. Their embeddings into hypercubes provide methods for computing the Wiener index and the Szeged index, while embeddings into the Cartesian product of trees lead to fast algorithms. A new method for computing the hyper-Wiener index of partial cubes in general, and of benzenoid graphs and trees in particular, is also presented.

1. Introduction

Graphs that can be isometrically embedded into a hypercube are called partial cubes. The structure of these graphs is well understood via characterizations of Djoković [**8**], Winkler [**31**] and Chepoi [**3**]. In addition, there are two algorithms of complexity $O(n^2 \log n)$ for recognizing these graphs, where n denotes the number of vertices of the graph considered. The algorithms are due to Aurenhammer, Hagauer [**2**] and Imrich, Klavžar [**18**], see also [**19**] for a survey on related algorithmic results.

Partial cubes have found several applications, in particular in the chemical graph theory. It was observed in [**22**] that benzenoid graphs are partial cubes. In this paper we wish to present the developments arising from this point of departure. We proceed as follows. In the rest of this section we recall the concepts needed later. In Sections 2 and 3 we survey results which were obtained using isometric embeddings of benzenoid graphs. Section 2 contains (theoretical) methods for computing the Wiener and the Szeged index of benzenoid graphs which in particular enable us to obtain expressions for the two indices of several families of benzenoid graphs. Section 3 contains linear algorithms for computing the two indices on benzenoid graphs. In Section 4 we propose a new method for computing the hyper-Wiener index of benzenoid graphs. At the end of the paper we also briefly mention the so-called scale embeddings, a generalization of isometric embeddings.

For a graph $G = (V(G), E(G))$ let $d_G(u, v)$ be the usual shortest path distance between vertices u and v of G. Given two connected graphs H and G, we say that H admits an *isometric embedding* into G if there exists a mapping

$$\iota : V(H) \to V(G)$$

1991 *Mathematics Subject Classification.* Primary 92E10, 05C12; Secondary 05C78, 68R10.
Supported by the Ministry of Science and Technology of Slovenia under the grant J1-0498-0101.

such that for all vertices $u, v \in V(H)$ we have
$$d_G(\iota(u), \iota(v)) = d_H(u, v)\,.$$
Clearly, ι is injective and maps edges to edges, thus H can be considered as an induced subgraph of G. We can also say that H is an *isometric subgraph* of G. An example of an isometric embedding is given in Fig. 1. We refer to [**9, 10, 30**] for more information on isometric embeddings of graphs.

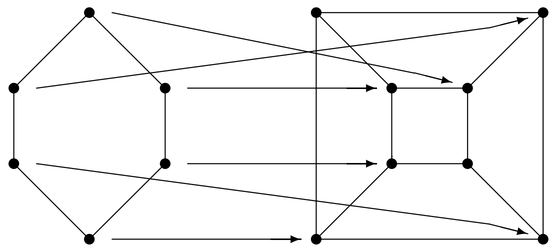


FIGURE 1. C_6 is an isometric subgraph of the 3-cube Q_3

The *Cartesian product* $G \Box H$ of graphs G and H is the graph with vertex set $V(G) \times V(H)$ and $(a, x)(b, y) \in E(G \Box H)$ whenever $ab \in E(G)$ and $x = y$, or $a = b$ and $xy \in E(H)$. The Cartesian product is commutative and associative. Hence we may write $G = G_1 \Box G_2 \Box \cdots \Box G_k$ for the Cartesian product of graphs $G_1, G_2, \ldots, G_k$. In this case, the vertex set of G is $V(G_1) \times V(G_2) \times \cdots \times V(G_k)$ and two vertices $(u_1, u_2, \ldots, u_k)$ and $(v_1, v_2, \ldots, v_k)$ are adjacent if they differ in exactly one position, say in ith, for which $u_i v_i$ is an edge of G_i. An example of the Cartesian product is given in Fig. 2 where we can see the Cartesian product of the path on four vertices P_4 with two copies of K_2.

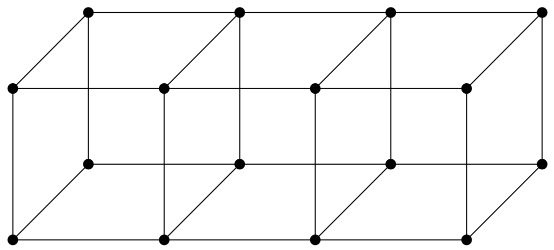


FIGURE 2. The Cartesian product $P_4 \Box K_2 \Box K_2$

The *n-cube* Q_n is the Cartesian product of n copies of the complete graph on two vertices K_2. In other words, if we set $V(K_2) = \{0, 1\}$, then the vertex set of Q_n consists of all words of length n over $\{0, 1\}$ and two such words are adjacent if they differ in exactly one position. A graph is called a *hypercube* if it is isomorphic to some n-cube.

The 3-cube, i.e. the graph $Q_3 = K_2 \Box K_2 \Box K_2$ can be seen on Fig. 1. Consider now the graph from Fig. 2. Since $K_2 \Box K_2 = Q_2$, the product graph can also be interpreted as $P_4 \Box (K_2 \Box K_2) = P_4 \Box Q_2$. Observe also that if we restrict P_4 to any of its three edges we find a copy of Q_3 in the product $P_4 \Box Q_2$.

A graph G is a *partial cube*, if there is an isometric embedding $\iota : V(G) \to V(Q_n)$ for some n. In other words, partial cubes are isometric subgraphs of hypercubes. We have seen already on Fig. 1 that C_6 is a partial cube. For another example see Fig. 3.

Another way of describing partial cubes is the following. Let $\Sigma = \{0, 1\}$ and let w_1 and w_2 be words of equal length over Σ. Then the *Hamming distance* between w_1 and w_2, $H(w_1, w_2)$, is the number of positions in w_1 and w_2 in which the two words differ. Then a graph G is a partial cube if and only if each vertex $v \in V(G)$ can be labeled by a word of fixed length, $\ell(v)$, such that for all $u, v \in V(G)$ we have

$$H(\ell(u), \ell(v)) = d_G(u, v)\,.$$

The partial cube from Fig. 3 is equipped with such a labeling.

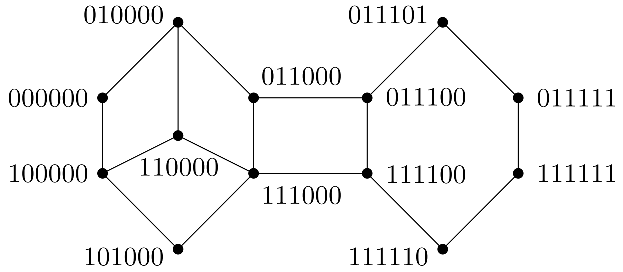


FIGURE 3. A partial cube with a corresponding labeling

Benzenoid graphs are graphs constructed as follows. Let H be the hexagonal (graphite) lattice and let Z be a circuit on it. Then a benzenoid system is formed by the vertices and edges of H, lying on Z and in the interior of Z. Note that the edge set of a benzenoid system can be partitioned into three classes of parallel edges. For more information on benzenoid graphs we refer to the book of Gutman and Cyvin [**11**].

2. Wiener and Szeged index of benzenoid graphs

The *Wiener index* $W(G)$ of a (connected) graph G is defined as

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d_G(u, v)\,.$$

The Wiener index, introduced in 1947 in [**29**], is one of the most important topological indices of chemical graphs. As many papers have already been written on this topic, we only refer to two recent surveys [**17, 26**] for more information on it.

For partial cubes we have the following result from [**22**]:

THEOREM 2.1. *Let G be a partial cube on n vertices embedded into the q-cube. For $i = 1, 2, \ldots, q$ let n_i be the number of vertices of G whose ith component of the embedding is equal to 1. Then*

$$W(G) = \sum_{i=1}^{q} n_i(n - n_i)\,.$$

In order to make Theorem 2.1 specific to benzenoid graphs, we need to recall the following concept. Let G be a benzenoid graph. A straight line segment $\mathbf{C}$ in the plane with end points P_1 and P_2 is called a *cut segment* if $\mathbf{C}$ is orthogonal to one of the three edge directions, each P_1 and P_2 is the center of an edge and the graph obtained from G by deleting all edges intersected by $\mathbf{C}$ has exactly two connected components. An *elementary cut* is the set of all edges intersected by a cut segment. Let $\mathcal{C}(G)$ be the set of all elementary cuts of G. For $C \in \mathcal{C}(G)$ let $n_1(C)$ and $n_2(C)$ be the number of vertices in the connected components of $G \setminus C$. As shown in [**14**], Theorem 2.1 refines as follows.

THEOREM 2.2. *For a benzenoid graph G we have*

$$W(G) = \sum_{C \in \mathcal{C}(G)} n_1(C) n_2(C)\,.$$

Theorem 2.2 provides a simple method for computing the Wiener index of benzenoid graphs by hand. For a simple example consider the molecular graph of naphthalene together with its 5 elementary cuts as shown in Fig. 4. Then the contribution of each of the cuts C_1, C_2, C_3 and C_4 is $3 \cdot 7$ and the contribution of C_5 is $5 \cdot 5$. Thus, the Wiener index of naphthalene is $4 \cdot (3 \cdot 7) + 5 \cdot 5 = 109$.

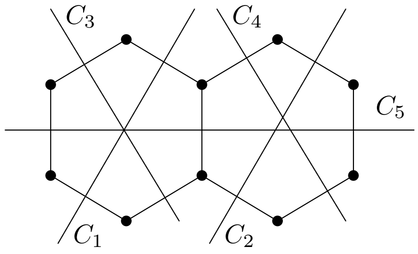


FIGURE 4. A benzenoid graph G with its elementary cuts

Theorem 2.2 can also be used to obtain expressions for the Wiener index of many classes of benzenoid graphs. For instance, it was shown in [**14**] that for the so-called coronene/circumcoronene series H_r we have:

COROLLARY 2.3. *For any $r \geq 1$ we have*

$$W(H_r) = \frac{1}{5}(164r^5 - 30r^3 + r)\,. \tag{2.1}$$

The finding of a general expression for $W(H_r)$ was, for a long time, considered as a special challenge in the theory of the Wiener index, but using Theorem 2.2 it becomes a routine matter. Corollary 2.3 was independently obtained by Shiu and Lam [**28**] with a much more complicated method. (In fact, formula (2.1) is the result of [**28**].)

Several formulas of type (2.1) are given in [**23**]. For instance, if $T(n,k)$ denotes the trapezium benzenoid graph with n columns and k rows of hexagons, then we have:

$$\begin{aligned} W(T(n,k)) \quad = \quad & \frac{4n^3(k^2+2k+1)}{3} - \frac{2n^2(k+1)(2k^2-8k-3)}{3} + \\ & \frac{2n(k^4-4k^3+6k^2+9k+1)}{3} - \frac{k(8k^4+35k^2-45k-28)}{30}\,. \end{aligned}$$

In particular, for $k = 1$ the above expression reduces to

$$W(P(n,1)) = \frac{1}{3}(16n^3 + 36n^2 + 26n + 3)\,,$$

which is the well-known formula for the Wiener index of polyacenes.

The Szeged index is a recently introduced topological index [**20**] and is defined as follows. For an edge $e = uv$ of a graph G let

$$W_{uv} = \{w \mid w \in V(G), d_G(w,u) < d_G(w,v)\}$$

and

$$W_{vu} = \{w \mid w \in V(G), d_G(w,v) < d_G(w,u)\}\,.$$

The *Szeged index* $Sz(G)$ of a graph G is defined as

$$Sz(G) = \sum_{uv \in E(G)} |W_{uv}|\,|W_{vu}|\,.$$

In [**13**] the following result similar to Theorem 2.2 was established:

THEOREM 2.4. *For a benzenoid graph G we have*

$$Sz(G) = \sum_{C \in \mathcal{C}(G)} |C|\, n_1(C) n_2(C)\,.$$

As in the case of the Wiener index, Theorem 2.4 can be used to obtain formulas for the Szeged index of classes of benzenoid graphs. For instance:

COROLLARY 2.5. *For any $k \geq 1$ we have*

$$Sz(H_k) = \frac{3}{2}k^2(36k^4 - k^2 + 1)\,.$$

3. Fast algorithms for W and Sz of benzenoid graphs

Let G be an arbitrary connected graph on n vertices and m edges. Then Mohar and Pisanski [**25**] showed that $W(G)$ can be computed in $O(mn)$ time. For the Szeged index the same result is due to Žerovnik [**32**]. In [**25**] it is also shown how to compute $W(G)$ in $O(n)$ time provided that G is a tree. In this section we present an $O(n)$ algorithm from [**6**] for computing $W(G)$ and $Sz(G)$ of a benzenoid graph G. Even faster algorithm of complexity $O(s)$ for the Wiener index of benzenoid graphs is proposed in [**7**], where s is the length of the outer cycle of a benzenoid graph considered. However, the last algorithm is of more theoretical than practical importance.

Let G be a benzenoid graph and let E_1, E_2, and E_3 denote the edges of G of a given direction. For $i = 1,2,3$ let G_i be the graph which is obtained from G be deleting all the edges of E_i. Define a graph T_i whose vertices are the connected components of G_i and two such components P' and P'' are adjacent in T_i if and only if there are vertices $u \in P'$ and $v \in P''$ which are end–vertices of an edge from E_i. Note that every T_i is a tree (the existence of a cycle in T_i would imply that G contains a non–hexagonal interior face). Then define the canonical emdedding

$$\alpha : V(G) \to V(T_1 \Box T_2 \Box T_3)$$

as

$$\alpha(v) = (P, Q, R)\,,$$

where P, Q, and R are the connected components of the graphs G_1, G_2, and G_3, respectively, sharing the vertex v. Chepoi [**4**] proved the following result:

THEOREM 3.1. *The canonical embedding map α provides an isometric embedding of a benzenoid graph G with n vertices into the graph $H = T_1 \Box T_2 \Box T_3$. The trees T_1, T_2, T_3 and the corresponding labels of the vertices of G can be computed in $O(n)$ time.*

In order to make use of the isometric map α we introduce the Wiener index of weighted graphs. A *weighted graph* (G, w) is a graph G together with a function $w : V(G) \to \mathbb{N}^+$. The Wiener index $W(G, w)$ of a weighted graph (G, w) is defined as

$$W(G,w) = \frac{1}{2} \sum_{u,v \in V(G)} w(u)\ w(v)\ d_G(u,v)\,.$$

Note that if all the weights are 1 then $W(G, w) = W(G)$.

The following result of [**6**] is the key to a fast algorithm for $W(G)$. We also include the proof since it reflects most of the tools needed.

THEOREM 3.2. *Let G be a benzenoid graph and let α be the canonical embedding of G into $T_1 \Box T_2 \Box T_3$. Then*

$$W(G) = W(T_1, w_1) + W(T_2, w_2) + w(T_3, w_3)\,.$$

PROOF. Let $V = V(G)$ and set $H = T_1 \Box T_2 \Box T_3$. For $u \in V$ let $\alpha(u) = (u_1, u_2, u_3)$. Then we have:

$$\begin{aligned}
W(G) &= \frac{1}{2} \sum_{u \in V} \sum_{v \in V} d_G(u,v) \\
&= \frac{1}{2} \sum_{u \in V} \sum_{v \in V} d_H(\alpha(u), \alpha(v)) && (3.1) \\
&= \frac{1}{2} \sum_{u \in V} \sum_{v \in V} \sum_{i=1}^{3} d_{T_i}(u_i, v_i) && (3.2) \\
&= \sum_{i=1}^{3} \left(\frac{1}{2} \sum_{u \in V} \sum_{v \in V} d_{T_i}(u_i, v_i) \right) \\
&= \sum_{i=1}^{3} \left(\frac{1}{2} \sum_{u_i \in T_i} \sum_{v_i \in T_i} w_i(u) w_i(v) d_{T_i}(u_i, v_i) \right) && (3.3) \\
&= \sum_{i=1}^{3} W(T_i, w_i). && (3.4)
\end{aligned}$$

In the above computation (3.1) holds because α is isometric. For (3.2) recall the following important and well-known property of the Cartesian product of graphs. If $u = (u_1, \ldots, u_k)$ and $v = (v_1, \ldots, v_k)$ are vertices of $G = G_1 \Box \cdots \Box G_k$ then $d_G(u, v) = \sum_{i=1}^{k} d_{G_i}(u_i, v_i)$. The equality (3.3) holds by the definition of the weighted trees (T_i, w_i). Finally, (3.4) is just the definition of the weighted Wiener index. $\Box$

By Theorem 3.2, a linear algorithm for computing $W(G)$ will be provided by a linear algorithm for computing the Wiener index of a weighted tree. This task was done implicitly by Mohar and Pisanski [**25**] and explicitly in [**6**], thus we can state:

THEOREM 3.3. *The Wiener index of a benzenoid graph on n vertices can be computed in $O(n)$ time.*

Moreover, along the same lines we obtain:

THEOREM 3.4. *The Szeged index of a benzenoid graph on n vertices can be computed in $O(n)$ time.*

4. Hyper-Wiener index

The hyper-Wiener index was in the case of trees introduced by Randić [**27**] and extended to all graphs by Klein, Lukovits and Gutman [**24**]. The *Hyper-Wiener index* $WW(G)$ of a graph G is defined as

$$WW(G) = \frac{1}{2} \sum_{u,v \in V(G)} \binom{d_G(u,v)+1}{2}$$

which can be rewritten as

$$WW(G) = \frac{1}{4} \sum_{u,v \in V(G)} d_G(u,v)^2 + \frac{1}{4} \sum_{u,v \in V(G)} d_G(u,v)\,. \tag{4.1}$$

We are going to develop a method for computing the hyper-Wiener index of partial cubes and thus in particular of benzenoid graphs and trees.

Let G be a partial cube on n vertices embedded into the q-cube and let ℓ be a corresponding Hamming labeling. For any $1 \le i, j \le q$ set

$$n_{ij}^{11} = \sum_{u \in V(G)} \ell_i(u)\ell_j(u)\,, \qquad n_{ij}^{00} = \sum_{u \in V(G)} (1-\ell_i(u))(1-\ell_j(u))\,,$$

$$n_{ij}^{10} = \sum_{u \in V(G)} \ell_i(u)(1-\ell_j(u))\,, \qquad n_{ij}^{01} = \sum_{u \in V(G)} (1-\ell_i(u))\ell_j(u)\,,$$

For instance, n_{ij}^{00} is the number of vertices of G whose ith and jth component of ℓ is equal to 0.

THEOREM 4.1. *Let G be a partial cube on n vertices embedded into the q-cube. Then*

$$WW(G) = W(G) + \sum_{i=1}^{q} \sum_{j=i+1}^{q} (n_{ij}^{11} n_{ij}^{00} + n_{ij}^{01} n_{ij}^{10})\,. \tag{4.2}$$

PROOF. As the second term of (4.1) is one half of the Wiener index, we need to concentrate on the first term only. Set $V = V(G)$ and for vertices u, v of G let $\delta_i(u,v)$ be 0 if ith components of $\ell(u)$ and $\ell(v)$ agree, and 1 otherwise. We have:

$$\begin{aligned}
\sum_{u\in V}\sum_{v\in V} d_G(u,v)^2 &= \sum_{u\in V}\sum_{v\in V}(H(\ell(u),\ell(v)))^2 \\
&= \sum_{u\in V}\sum_{v\in V}(\sum_{i=1}^{q}\delta_i(u,v))^2 \\
&= \sum_{u\in V}\sum_{v\in V}\sum_{i=1}^{q}\sum_{j=1}^{q}\delta_i(u,v)\delta_j(u,v) \\
&= \sum_{i=1}^{q}\sum_{j=1}^{q}(\sum_{u\in V}\sum_{v\in V}\delta_i(u,v)\delta_j(u,v)) \\
&= \sum_{i=1}^{q}\sum_{u\in V}\sum_{v\in V}\delta_i(u,v)\delta_i(u,v) + \sum_{i=1}^{q}\sum_{\substack{j=1\\ j\neq i}}^{q}\sum_{u\in V}\sum_{v\in V}\delta_i(u,v)\delta_j(u,v) \\
&= \sum_{i=1}^{q}\sum_{u\in V}\sum_{v\in V}\delta_i(u,v) + \sum_{i=1}^{q}\sum_{\substack{j=1\\ j\neq i}}^{q}\sum_{u\in V}\sum_{v\in V}\delta_i(u,v)\delta_j(u,v) \\
&= 2W(G) + 2\sum_{i=1}^{q}\sum_{\substack{j=1\\ j\neq i}}^{q}(\frac{1}{2}\sum_{u\in V}\sum_{v\in V}\delta_i(u,v)\delta_j(u,v)) \\
&= 2W(G) + 2\sum_{i=1}^{q}\sum_{\substack{j=1\\ j\neq i}}^{q}(n_{ij}^{11}n_{ij}^{00} + n_{ij}^{01}n_{ij}^{10}) \\
&= 2W(G) + 4\sum_{i=1}^{q}\sum_{j=i+1}^{q}(n_{ij}^{11}n_{ij}^{00} + n_{ij}^{01}n_{ij}^{10})
\end{aligned}$$

Inserting this expression into (4.1) yields the result. □

In the case of benzenoid graphs, Theorem 4.1 provides a particular simple procedure for computing the hyper-Wiener index. We compute the Wiener index and for the second term of (4.2) we proceed as follows. Let C_1 and C_2 be two elementary cuts of a benzenoid graph G. There are two different cases, as shown in Fig. 5. With a, b, c and d we denote the number of vertices in the corresponding parts of G. Then the contribution of the pair C_1, C_2 to (4.2) is $ab + cd$ in the first case and ab in the second one.

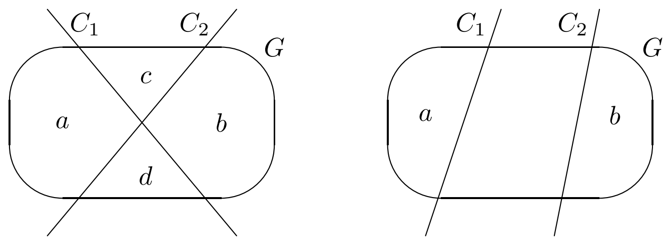


FIGURE 5. Different positions between two elementary cuts

For a concrete example consider the benzenoid graph (naphthalene) from Fig. 4 together with its elementary cuts C_1, C_2, C_3, C_4 and C_5. The contributions of pairs of cuts

$C_1, C_2;\ C_1, C_3;\ C_1, C_4;\ C_1, C_5;\ C_2, C_3;$
$C_2, C_4;\ C_2, C_5;\ C_3, C_4;\ C_3, C_5;\ C_4, C_5$

are, respectively:

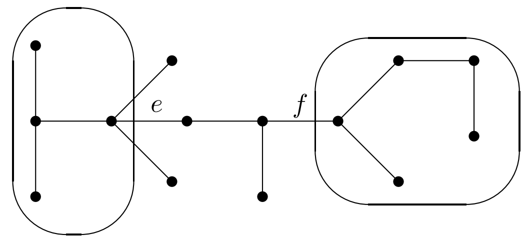
$$3 \cdot 3 + (1 \cdot 1 + 2 \cdot 6) + 3 \cdot 3 + (2 \cdot 4 + 1 \cdot 3) + 3 \cdot 3 +$$
$$(1 \cdot 1 + 2 \cdot 6) + (1 \cdot 3 + 2 \cdot 4) + (1 \cdot 1 + 2 \cdot 6) + 3 \cdot 3 + (1 \cdot 3 + 2 \cdot 4) = 106.$$

Therefore $WW(G) = W(G) + 106 = 109 + 106 = 215$.

As already mentioned, trees are partial cubes as well. For trees, the formula (4.2) reduces to

$$WW(T) = W(T) + \sum_{e \in E(T)} \sum_{\substack{f \in E(T) \\ f > e}} n_1(e, f) \cdot n_2(e, f)$$

where $n_1(e, f)$ and $n_2(e, f)$ are the number of vertices in the two "extremal" connected components in the graph $T \setminus \{e, f\}$, see Fig. 6. More precisely, a pair of cuts in a tree is just a pair of edges, and its contribution to (4.2) is always the second case from Fig. 5. We don't want to go into more details in this particular case, because this was previously observed by Aringhieri, Hansen and Malcucelli [**1**]. Moreover, in [**1**] implementation details are also provided to obtain a linear algorithm for computing the hyper-Wiener index of a tree.



$n_1(e, f) = 4$ $\qquad$ $n_2(e, f) = 5$

FIGURE 6. A tree and the two extremal components with respect to e, f

5. Concluding remarks

Isometric embeddings were also applied by Gutman, Khadikar and Khaddar [**12**] in the study of benzenoid graphs containing a linear polyacene fragment as well as in [**15, 16, 21**] for the study of phenylenes.

A generalization of isometric embeddings is provided with the following concept. Let $\lambda \in \mathbb{N}$ and let G and H be two graphs. Then we say that H is *scale λ embeddable* into G if there exists a mapping

$$\iota : V(H) \to V(G)$$

such that for all vertices $u, v \in V(H)$ we have

$$d_G(\iota(u), \iota(v)) = \lambda d_H(u, v)\,.$$

Note that if $\lambda = 1$ then we are back to the isometric embeddings. A graph is an L_1-*graph* if it admits a scale embedding into a hypercube. Chepoi, Deza and Grishukhin [**5**] extended Theorem 2.1 to the class of all L_1-graphs. Their theorem is important for non-bipartite graphs, since in the bipartite case the L_1-graphs coincide with the partial cubes. In the non-bipartite case the class of L_1-graphs is a rich class of graphs containing many chemical graphs and thus a lot of work is waiting to be done.

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