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Exploring the Strong Metric Dimension of Hollow Coronoid Structures: Applications and Implications

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Abstract

Coronoid systems are actually geometric arrangements of six-sided benzenoids in hexagonal form. Coronoid systems are organic chemical structures, that fall into two categories: primitive and catacondensed coronoids. Many researchers from various fields have an interest in the mathematical analysis of chemicals. Graph theory played an important role in studying chemical structures by transforming them into a graph. The strong metric dimension is one of the main parameter of graph theory. Consider a connected graph G, a vertex u strongly resolves a pair (x, y) of vertices if either x lies on a shortest path between $u - y$ or y lies on a shortest path between $u - x$. The set S is referred as the strong resolving set of G if any vertex in S can strongly resolve every pair of distinct vertices in G. The minimum cardinality of such set S is known as the strong metric dimension of G.

Keywords: metric, metric dimension, strong metric dimension, strong resolving graph, vertex cover number.

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1|Introduction

Graph theory is a field of study in mathematics concerned with network structure and object interaction. Graph theory has numerous applications far beyond mathematics. Some of the significant applications of graph theory are in aviation networks, map directions, algorithms used by search engines, traffic signals, solving sudoku's puzzles, epidemiology, and many more. Chemical graph theory is recognized as a wide rang field that combines mathematics and chemistry. It focuses on using mathematics to comprehend chemical structures by transforming them into graphs. Chemical structures are transformed into graphs by turning atoms into vertices and lines joining atoms into edges. Different parameters captivate the attention of many researchers to study chemical structures, and the identification of vertices is one of them.

The challenge of uniquely identifying the vertices in a graph attracted many researchers because of its widespread applications. Many researchers worked on uniquely identifying the vertices by using different useful concepts of graph theory including coloring, labeling, covering of vertices, and by defining the metric on graphs.

Vertex identification by defining metrics on graphs has numerous applications in chemical graph theory and computer networks including network discovery [5], navigation of robots [20], game strategies by using resolving sets in a hamming graph [12], to study digital images, resolving sets have been proposed in triangular, rectangular, and hexagonal grids [37] and coins weighing problems [46]. Afterwards, many researchers extended the idea of metric identification of vertices by determining different parameters of metric dimension including fractional [4], double [10], independent [11], weighted [14], k-metric [16], solid [17], local [40], mixed [19], connected [42] and the strong metric dimension [45].

Consider a connected graph G with vertex set $V(G)$. A path is a sequence of non-repeated vertices connected through edges. Distance is defined as the length of the shortest path connecting two vertices ψ, χ and denoted by $d(\psi, \chi)$. Inspired by the issue of uniquely identifying the vertices of a graph, the idea of locating sets was presented by Slater in [47]. After that Harary and Melter independently introduced a similar idea in [18] where they name locating sets as resolving sets. We use the term resolving sets throughout our work.

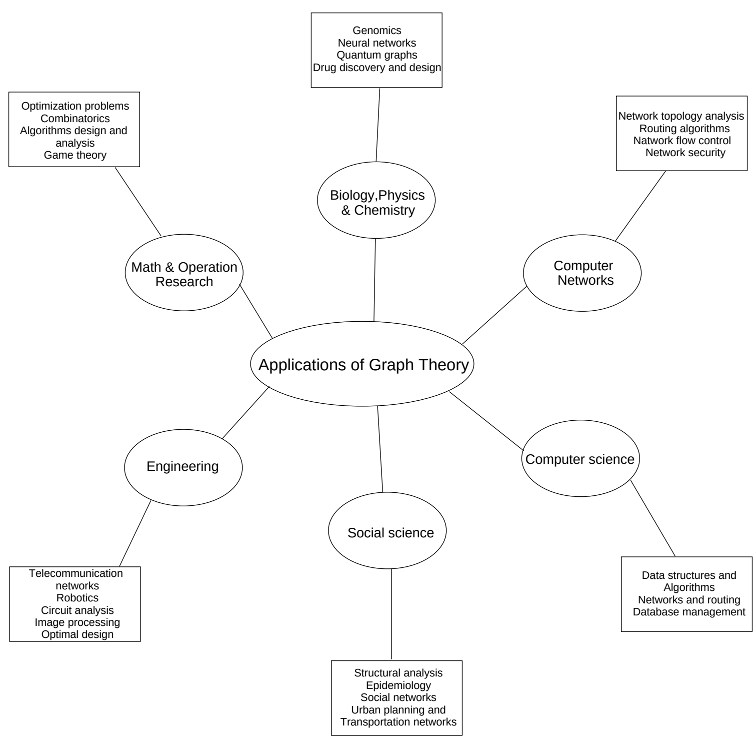

Figure 1. Applications of Graph Theory

A pair of vertices $\xi, \zeta \in V(G)$ resolves by a vertex $x \in V(G)$ if distance between ξ and x is not equal to distance between ζ and x mathematically $d(\xi, x) \neq d(x, \zeta)$. A set of vertices W in G said to be resolving set of G if each pair of unique vertices in G can be resolved by any vertex in W. Cardinality of minimum resolving set is called the metric dimension of G.

The strong metric dimension is more defined parameter than the metric dimension was originally introduced in [45] by Sebö and Tannier and further studied by numerous researchers in many papers. That is a vertex $x \in V(G)$ strongly resolves two vertices $a, b \in V(G)$ if a shortest path between (x, a) contains b or a shortest path between (x, b) contains a. A set of vertices $W \subseteq V(G)$ is called strong resolving set of G if each pair of distinct vertices of G is strongly resolved by any vertex in W the minimum cardinality of overall strong resolving sets of G is called the strong metric dimension of G, denoted as $Sdim(G)$ [45].

After Sebö and Tannier many researchers extend the study of the strong metric dimension. The concept of strong metric dimension has been studied in some convex polytopes in [24] and in [43], in convex plane graph [1], in some famous graphs [27], in hamming graphs [25], in sunflower, friendship, helm and t-fold wheel graphs [26], in direct product graphs [28], in generalized sierpiriski graph [15], in power graph of finite groups [34], in anti-prism and king graphs [38], in zero divisor graph of rings [6], in distance hereditary graphs [35], in some graphs and their compliment [50], in cartesian sum graphs [31], in windmill graph K_n^m, sun graph S_n and mobius ladder graphs M_n [49], in generalized butterfly, starbarbell, and $C_m \odot P_n$ graphs [36], in crossed prism [51].

Cartesian product, direct product, rooted product, lexicographic product, strong product and corona product are some common graph products, also called standard products. For such classes of graphs a lot of graphs invariant are studied to calculate their exact values or to predicting their action based on the factor graphs. The strong metric dimension of the graph's products also has been investigated in the following published articles. In some families of direct product graph [28], rooted product graphs [30], lexicographic product [29], strong product, corona product, graphs and digraphs, cartesian and direct product of graph has been investigated in [32, 33, 39, 41].

In this article, we investigate the strong metric dimension of the hollow coronoid structure. Different variants of metric dimension have been studied on hollow coronoid structures in the following articles. Metric and fault-tolerant metric dimension in [21], edge metric and fault-tolerant edge metric dimension in [22] and mixed metric dimension of hollow coronoid in [23]. Vertex identification through the definition of a metric on a graph has many applications in computer networks [52] and chemical graph theory [53, 54], such as network discovery, robot navigation, the study of digital images, resolving sets in triangular, rectangular, and hexagonal grids, and coin weighing problems. Subsequently, numerous scholars expand upon the concept of metric vertex identification by ascertaining various metric dimension characteristics, such as fractional, double, independent, weighted, k-metric, solid, local, mixed, linked, and strong metric dimensions. Additional uses include resource allocation in transportation networks [55, 56], researching the dissemination of information in social networks [57], identifying anomalies in cyber-physical systems, and examining epidemic trends in epidemiology.

In conclusion, this work creates a wealth of opportunities for additional theoretical research on the metric dimensions of chemical structures, algorithm development, and practical applications. Expanding upon these discoveries may reveal novel perspectives at the nexus of graph theory, metric geometry, and chemistry[58].

2|Working approach

Now we are formalizing all the necessary terminology and notations that we will use throughout the article. Let G denote a connected graph shown in Figure 2, where the vertex set of G is denoted by $V(G)$ and the edge set of G by $E(G)$. In a graph G if two vertices m, n share an common edge between them then they are called adjacent vertices and denoted by $m \sim n$. A vertex set containing all the adjacent vertices of m is called neighborhood of m and denoted as $N(m)$, sometimes $N(m)$ is called open neighborhood of m. A vertex ϑ strongly resolves a pair (ϱ, φ) of distinct vertices if either $d(\vartheta, \varrho) = d(\vartheta, \varphi) + d(\varphi, \varrho)$ or $d(\vartheta, \varphi) = d(\vartheta, \varrho) + d(\varrho, \varphi)$. In our work we take help from the following result of Kratica *et al.* [24] to find which pair of distinct vertices cannot be strongly resolves by any vertex of G.

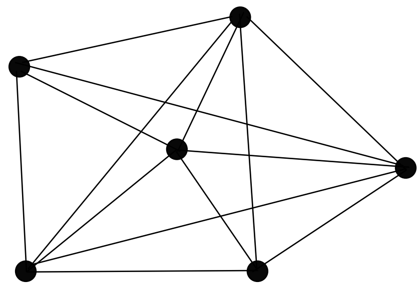

FIGURE 2. A Graph

Lemma 1. [24] Let (γ, δ) be a pairs of vertices in a connected graph G such that

$$d(\gamma, \delta) \geq d(\omega, \delta)\ \forall\ \omega \in N(\gamma) \quad \textit{and} \quad d(\gamma, \delta) \geq d(\omega, \gamma)\ \forall\ \omega \in N(\delta) \tag{1}$$

Then there is no vertex in $V(G) - \{\gamma, \delta\}$ which performs the strong metric identification for the pair (γ, δ).

To examine the strong metric dimension of hollow coronoid we use the concept of strong resolving graph which was proposed by Ollermann and Fransen in [39]. If a pair $(\xi, \zeta) \in V(G)$ of distinct vertices satisfied both the condition in (1) then the vertices are said to be mutually maximally distant, denoted as $\xi MMD\zeta$. The strong resolving graph of a graph G is a graph G_{SR} with vertex set contained all MMD vertices and there is an edge between two vertices if and if they are MMD with each others in original graph G.

If $W \subseteq V(G)$ then W is a vertex cover of G if every edge in G is incident with some vertex of W and the cardnality of minimum vertex cover of G is called vertex cover number or covering number of G denoted by $\tau(G)$ [48]. In the following theorem Ollerman and Fransen established a relationship between covering number of strong resolving graph G_{SR} and the strong metric dimension.

Theorem 2. [39] For any connected graph G,

$$sdim(G) = \tau(G_{SR}).$$

Throughout our work notation K_l represent complete graph and C_l represent cycle graph. We have the following remark according to the definition of vertex cover number.

Remark 3. *Assume that G is a connected graph, then*

(1) *If G is complete graph K_l on $l \geq 2$ vertices, then $\tau(G) = l - 1$.*

(2) *If G is cycle graph on $l \geq 3$ vertices, then $\tau(G) = \lceil \frac{l}{2} \rceil$.*

3|Construction of hollow coronoid $HC(x, y, z)$

The name coronoid was coined in 1987 [9] due to its potential link with benzenoid. Since coronoid is a benzenoid with a central hole. A particular kind of polyhex system having origins in organic chemistry is referred to as a "coronoid". Hollow coronoid contained six sides x, y, z, x', y', z' as shown in Figure 3. It drives from the catacondensed coronoids and is a member of the primitive coronoid [7].

A new type of hollow coronoid structure has been identified in [44]. In [8, 2, 3] author discussed mathematical study of coronoid and related structures. [13] describes the relationship between the hollow coronoid and the polyhex..

Our study examines a six-sided $x = x' = y = y' = z = z'$ hollow coronoid, however the three sides (x, y, z) are symmetric to the other three sides (x', y', z'). Hollow coronoid label as $HC(x, y, z)$ with $x, y, z \geq 2$. Hollow coronoid contained total $8(x + y + z - 3)$ vertices and $10(x + y + z - 3)$ edges from which $4(x + y + z - 3)$ are

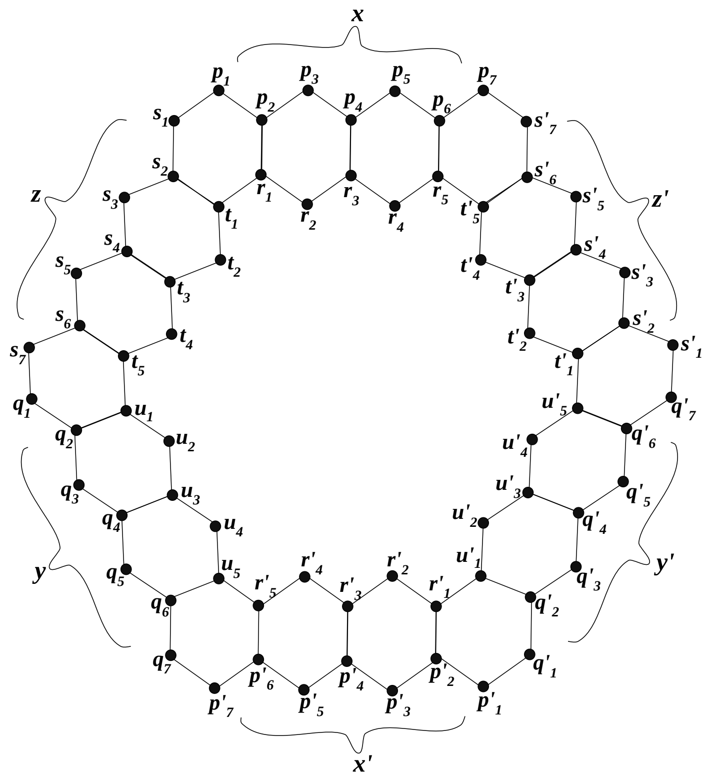

FIGURE 3. Hollow Coronoid $x = y = z = 4$

of degree 2 and the same number of vertices with degree 3. The description of the vertex and edge set of a hollow coronoid structure $HC(x, y, z)$ is given as:

$$\begin{aligned}
V(HC(x,y,z)) = &\{p_i, p_i' : 1 \le i \le 2x-1\} \cup \{s_i, s_i' : 1 \le i \le 2z-1\} \\
&\cup \{q_i, q_i' : 1 \le i \le 2y-1\} \cup \{r_i, r_i' : 1 \le i \le 2x-3\} \\
&\cup \{t_i, t_i' : 1 \le i \le 2z-3\} \cup \{u_i, u_i' : 1 \le i \le 2y-3\}, \\
E(HC(x,y,z)) = &\left\{p_i p_{i+1}, p_i' p_{i+1}' : 1 \le i \le 2x-2\right\} \cup \left\{q_i q_{i+1}, q_i' q_{i+1}' : 1 \le i \le 2y-2\right\} \\
&\cup \left\{s_i s_{i+1}, s_i' s_{i+1}' : 1 \le i \le 2z-2\right\} \cup \left\{r_i r_{i+1}, r_i' r_{i+1}' : 1 \le i \le 2x-4\right\} \\
&\cup \left\{u_i u_{i+1}, u_i' u_{i+1}' : 1 \le i \le 2y-4\right\} \cup \left\{t_i t_{i+1}, t_i' t_{i+1}' : 1 \le i \le 2z-4\right\} \\
&\cup \left\{t_i s_{i+1}, t_i' s_{i+1}' : 1 \le i(odd) \le 2z-3\right\} \cup \left\{r_i p_{i+1}, r_i' p_{i+1}' : 1 \le i(odd) \le 2x-3\right\} \\
&\cup \left\{u_i q_{i+1}, u_i' q_{i+1}' : 1 \le i(odd) \le 2y-3\right\} \cup \left\{q_1 s_{2z-1}, q_i' s_{2z-1}', s_1 p_1, s_{2z-1}' p_{2x-1}'\right\} \\
&\cup \left\{p_1' q_1', p_{2x-1}' q_{2y-1}, t_{2z-3} u_1, t_1' u_{2y-3}, t_1 r_1, t_{2z-3}' r_{2x-3}, u_1' r_1', r_{2x-3}' u_{2y-3}\right\}.
\end{aligned}$$

4|Results

Lemma 4. *The strong resolving graph of $HC(x, y, z)$ where $x = y = z \ge 2$ is isomorphic to $(x+y+z-6)K_4+3C_4$.*

Proof: In order to construct $HC(x,y,z)_{SR}$ we find each pair (u,v) of vertices in $HC(x,y,z)$ such that $uMMDv$. For the MMD pairs of vertices consider the table 1 It follows according to Table 1 all pairs of vertices satisfies

TABLE 1. MMD pairs of vertices in $HC(x,y,z)$

(x,y)	$d(x,y)$	$d(x,a)\ \forall\ a \in N(y)$	$d(b,y)\ \forall\ b \in N(x)$
(p_{i+1}, r_i) for $2 \leq i(even) \leq 2x-4$	$d(p_{i+1}, r_i) = 3$	$d(p_{i+1}, a) = 2$	$d(b, r_i) = 2$
(p'_{i+1}, r'_i) for $2 \leq i(even) \leq 2x-4$	$d(p'_{i+1}, r'_i) = 3$	$d(p'_{i+1}, a) = 2$	$d(b, r'_i) = 2$
(s_{i+1}, t_i) for $2 \leq i(even) \leq 2z-4$	$d(s_{i+1}, t_i) = 3$	$d(s_{i+1}, a) = 2$	$d(b, t_i) = 2$
(s'_{i+1}, t'_i) for $2 \leq i(even) \leq 2z-4$	$d(s'_{i+1}, t'_i) = 3$	$d(s'_{i+1}, a) = 2$	$d(b, t'_i) = 2$
(q_{i+1}, u_i) for $2 \leq i(even) \leq 2y-4$	$d(q_{i+1}, u_i) = 3$	$d(q_{i+1}, a) = 2$	$d(b, u_i) = 2$
(q'_{i+1}, u'_i) for $2 \leq i(even) \leq 2y-4$	$d(q'_{i+1}, u'_i) = 3$	$d(q'_{i+1}, a) = 2$	$d(b, u'_i) = 2$
(r_i, r'_i) for $2 \leq i(even) \leq 2x-4$	$d(r_i, r'_i) = 6x-9$	$d(r_i, a) = 6x-10$	$d(b, r'_i) = 6x-10$
(t_i, u'_i) for $2 \leq i(even) \leq 2z-4$	$d(t_i, u'_i) = 6z-9$	$d(t_i, a) = 6z-10$	$d(b, u'_i) = 6z-10$
(u_i, t'_i) for $2 \leq i(even) \leq 2y-4$	$d(u_i, t'_i) = 6y-9$	$d(u_i, a) = 6y-10$	$d(b, t'_i) = 6y-10$
(p_i, r'_{i-1}) for $3 \leq i(odd) \leq 2x-3$	$d(p_i, r'_{i-1}) = 6x-8$	$d(p_i, a) = 6x-9$	$d(b, r'_{i-1}) = 6x-9$
(s_i, u'_{i-1}) for $3 \leq i(odd) \leq 2z-3$	$d(s_i, u'_{i-1}) = 6z-8$	$d(s_i, a) = 6z-9$	$d(b, u'_{i-1}) = 6z-9$
(q_i, t'_{i-1}) for $3 \leq i(odd) \leq 2y-3$	$d(q_i, t'_{i-1}) = 6y-8$	$d(q_i, a) = 6y-9$	$d(b, t'_{i-1}) = 6y-9$
(p'_i, r_{i-1}) for $3 \leq i(odd) \leq 2x-3$	$d(p'_i, r_{i-1}) = 6x-8$	$d(p'_i, a) = 6x-9$	$d(b, r_{i-1}) = 6x-9$
(s'_i, u_{i-1}) for $3 \leq i(odd) \leq 2z-3$	$d(s'_i, u_{i-1}) = 6z-8$	$d(s'_i, a) = 6z-9$	$d(b, u_{i-1}) = 6z-9$
(q'_i, t_{i-1}) for $3 \leq i(odd) \leq 2y-3$	$d(q'_i, t_{i-1}) = 6y-8$	$d(q'_i, a) = 6y-9$	$d(b, t_{i-1}) = 6y-9$
(p_i, p'_j), $i \neq j$ for $i,j \in \{1, 2x-1\}$	$d(p_i, p'_j) = 4x-1$	$d(p_i, a) = 4x-2$	$d(b, p'_j) = 4x-2$
(s_i, q'_j), $i \neq j$ for $i,j \in \{1, 2z-1\}$	$d(s_i, q'_j) = 4z-1$	$d(s_i, a) = 4z-2$	$d(b, q'_j) = 4z-2$
(q_i, s'_j), $i \neq j$ for $i,j \in \{1, 2y-1\}$	$d(q_i, s'_j) = 4y-1$	$d(q_i, a) = 4y-2$	$d(b, s'_j) = 4y-2$

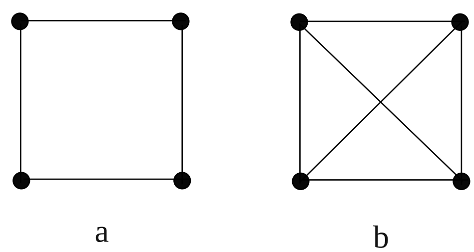

FIGURE 4. (a) is a C_4 and (b) is a K_4

both the condition in (1) so, vertices in each pairs are MMD with each other.

Now, consider the pair (p_i, p'_i) for $1 \leq i(odd) \leq 2x-1$. Note that,

$$d(p_i, p'_i) = \begin{cases} 6x-7 & , \quad 3 \leq i(odd) \leq 2x-3, \\ 6x-5 & , \quad i = \{1, 2x-1\}. \end{cases}$$

and for $a \in N(p'_i),\ b \in N(p_i)$

$$d(p_i, a) = d(b, p'_i) = \begin{cases} 6x-8 & , \quad 3 \leq i(odd) \leq 2x-3, \\ 6x-6 & , \quad i = \{1, 2x-1\}. \end{cases}$$

the pair (p_i, p'_i) satisfied both the conditions in (1) as $d(p_i, a) = d(b, p'_i) \leq d(p_i, p'_i)$. So, $p_i MMD p'_i$ with each other.

Now, consider the pair (q_i, s'_i) for $1 \leq i(odd) \leq 2y-1$. Note that,

$$d(q_i, s'_i) = \begin{cases} 6y-7 & , \quad 3 \leq i(odd) \leq 2y-3, \\ 6y-5 & , \quad i = \{1, 2y-1\}. \end{cases}$$

and for $a \in N(s_i'),\ b \in N(q_i)$

$$d(q_i,a) = d(b,s_i') = \begin{cases} 6y-8 & , \quad 3 \leq i(odd) \leq 2y-3, \\ 6y-6 & , \quad i = \{1, 2y-1\}. \end{cases}$$

the pair (q_i, s_i') satisfied both the conditions in (1) as $d(q_i,a) = d(b,s_i') \leq d(q_i,s_i')$. So, $q_i MMD s_i'$ with each other.

Now, consider the pair (s_i, q_i') for $1 \leq i(odd) \leq 2z-1$. Note that,

$$d(s_i,q_i') = \begin{cases} 6z-7 & , \quad 3 \leq i(odd) \leq 2z-3, \\ 6z-5 & , \quad i = \{1, 2z-1\}. \end{cases}$$

and for $a \in N(q_i'),\ b \in N(s_i)$

$$d(s_i,a) = d(b,q_i') = \begin{cases} 6z-8 & , \quad 3 \leq i(odd) \leq 2z-3, \\ 6z-6 & , \quad i = \{1, 2z-1\}. \end{cases}$$

the pair (s_i, q_i') satisfied both the conditions in (1) as $d(s_i,a) = d(b,q_i') \leq d(s_i,q_i')$. So, $s_i MMD q_i'$ with each other. We construct the following vertex and edge set of $HC(x,y,z)_{SR}$ from MMD pairs of vertices in $HC(x,y,z)$.

$$\begin{aligned}
V(HC(x,y,z)_{SR}) &= \{p_1, p_3, \ldots, p_{2x-1}, p_1^{'}, p_3^{'}, \ldots, p_{2x-3}^{'}\} \cup \{s_1, s_3, \ldots, s_{2z-1}, s_1^{'}, s_3^{'}, \ldots, s_{2z-3}^{'}\} \\
&\cup \{q_1, q_3, \ldots, q_{2y-1}, q_1^{'}, q_3^{'}, \ldots, q_{2y-3}^{'}\} \cup \{r_2, r_4, \ldots, r_{2x-4}, r_2^{'}, r_4^{'}, \ldots, r_{2x-4}^{'}\} \\
&\cup \{t_2, t_4, \ldots, t_{2z-4}, t_2^{'}, t_4^{'}, \ldots, t_{2z-4}^{'}\} \cup \{u_2, u_4, \ldots, u_{2y-4}, u_2^{'}, u_4^{'}, \ldots, u_{2y-4}^{'}\} \\
E(HC(x,y,z)_{SR}) &= \{p_1 \sim p_1^{'}, p_3 \sim p_3^{'}, \ldots, p_{2x-1} \sim p_{2x-1}^{'}\} \cup \{s_1 \sim q_1^{'}, s_3 \sim q_3^{'}, \ldots, s_{2z-1} \sim q_{2y-1}^{'}\} \\
&\cup \{q_1 \sim s_1^{'}, q_3 \sim s_3^{'}, \ldots, q_{2y-1} \sim s_{2z-1}^{'}\} \cup \{p_3 \sim r_2^{'}, p_5 \sim r_4^{'}, \ldots, p_{2x-3} \sim r_{2x-4}^{'}\} \\
&\cup \{s_3 \sim u_2^{'}, s_5 \sim u_4^{'}, \ldots, s_{2z-3} \sim u_{2y-4}^{'}\} \cup \{q_3 \sim t_2^{'}, q_5 \sim t_4^{'}, \ldots, q_{2y-3} \sim t_{2z-4}^{'}\} \\
&\cup \{r_2 \sim r_2^{'}, r_4 \sim r_4^{'}, \ldots, r_{2x-4} \sim r_{2x-4}^{'}\} \cup \{t_2 \sim u_2^{'}, t_4 \sim u_4^{'}, \ldots, t_{2z-4} \sim u_{2y-4}^{'}\} \\
&\cup \{u_2 \sim t_2^{'}, u_4 \sim t_4^{'}, \ldots, u_{2y-4} \sim t_{2z-4}^{'}\} \cup \{r_2 \sim p_3^{'}, r_4 \sim p_5^{'}, \ldots, r_{2x-4} \sim p_{2x-3}^{'}\} \\
&\cup \{t_2 \sim q_3^{'}, t_4 \sim q_5^{'}, \ldots, t_{2z-4} \sim q_{2y-3}^{'}\} \cup \{u_2 \sim s_3^{'}, u_4 \sim s_5^{'}, \ldots, u_{2y-4} \sim s_{2z-3}^{'}\} \\
&\cup \{p_1 \sim p_{2x-1}^{'}, p_{2x-1} \sim p_1^{'}, s_1 \sim q_{2y-1}^{'}, s_{2z-1} \sim q_1^{'}, q_1 \sim s_{2z-1}^{'}, q_{2y-1} \sim s_1^{'}\}.
\end{aligned}$$

□

Theorem 5. *For $x = y = z \geq 2$, $sdim(HC(x,y,z)) = 3(x+y+z) - 12$.*

Proof: As strong resolving graph of $HC(x,y,z)$ is isomorphic to $(x+y+z-6)K_4 + 3C_4$, by Remark 3 a minimum vertex cover W of the graph $HC(x,y,z)_{SR}$ must contains 3 vertices from each copies of K_4 and 2 vertices from each copies of C_4. So, by Theorem 2 $sdim(HC(x,y,z)) = \tau(HC(x,y,z)) = |W| = 3(x+y+z) - 12$. □

5|Application and Case Study:

5.1|Fault Diagnosis in Chemical Process Plants

Reactors, heat exchangers, distillation columns, storage tanks, and other associated equipment are just a few of the complex networks that make up chemical process plants. Ensuring safety, optimizing effectiveness, and minimizing financial losses require close observation of each unit's proper operation and quick identification of malfunctions or unusual behaviors. A helpful method is for the visualizing a process plant's network topology is an application of the graph theory. To look at these individual units are portrayed as vertices in this depiction, as well as the physical connections among them are shown as edges in the results. Also to analyzing with these networks and the developing efficient defect diagnosis methods can be very accomplished by implementing the concepts from graph theory such as metric dimensions and the application of these topics.

We can show it by an example, consider to look at a specific section of a processing plant that makes aspirin, or we can also take as acetylsalicylic acid. Reactors, product separators, waste streams, recycle streams, and product storage tanks are typical parts of this area. Now we can see that as thinking of this portion as a hollow coronoid graph, as well as with the reactor, separator, and tank as the longer sides and the recycle/waste streams as the shorter ones, one can create an organized representation of it in the application process. Now for fully monitor the network as a whole of the system, here we can determine the lowest set of units (vertices) by determining the graph's strong metric dimension for this application. for all these units which are essentially important measuring points that are employed to spot anomalies or deviations from standard operating parameters in this system. We can see that for the time, the data from sensors at these critical vertices, like reactor temperature or product tank level, that depart from predicted values suggest a similarly malfunction in the relevant units for this particular application.

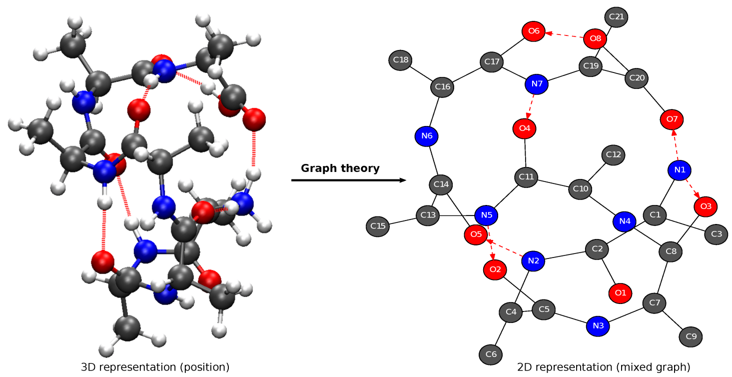

Figure 5. A single 3D depiction on the left and the corresponding 2D MolGraph on the right are snapshots from a peptide trajectory in the gas phase.

Resolving all other unit pairings requires the vertices for the reactor, separator, and product tank, which together provide the strong metric basis. The dimensions obtained from this study make it easier to determine exactly how few monitoring points are needed for aspirin plant subsection graphs of different sizes. By intelligently situating sensors, this optimization helps to maximize problem diagnosis capabilities while minimizing resource consumption. The topological structure of chemical graphs can be efficiently captured to determine the best places to place sensors by utilizing the strong metric dimension metric.

This real-world use highlights the value of learning about metric dimensions in chemical graph theory for process monitoring, risk mitigation, and troubleshooting in the chemical industry. Theoretical knowledge acquired from these types of analysis is crucial for optimizing operational resilience through improved fault diagnosis techniques and sensor placement decisions.

5.2|Results and Discussions

The utilization of graph theory principles, specifically with regard to metric dimensions, in fault diagnosis for chemical process plants—such as those engaged in the production of aspirin or acetylsalicylic acid—has shown to result in notable improvements in terms of safety, efficiency, and loss mitigation.

5.3|Graph Representation and Analysis

- For instance, data from sensors at these critical vertices, such as reactor temperature or product tank level, that depart from predicted values suggest a likely malfunction in the relevant units.

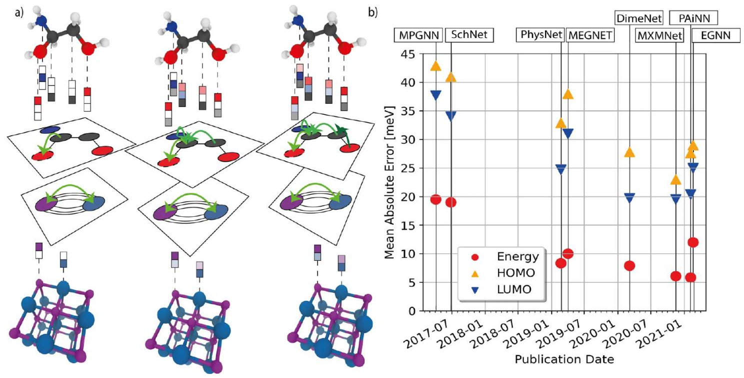

FIGURE 6. A schematic representation of the message passing process in crystalline materials and molecules. b Benchmark for QM9. Since 2017, the mean absolute error of the predicted energies for several GNN models has been represented by internal (red circles), lowest unoccupied molecular orbital (LUMO, inverted blue triangles), and highest occupied molecular orbital (HOMO, orange triangles).

- Unit interdependencies could be clearly illustrated by using hollow coronoid diagrams to visualize specific subsections, like the one on aspirin production.

5.4|Identification of Critical Measurement Points

- The smallest set of crucial measurement points required for closely observing the entire network might be found by locating the strong metric dimension.
- Important components such as the reactor, product separator, and product storage tank have made it feasible to address possible flaws or unusual behaviors throughout the network.

5.5|Optimization of Sensor Placement

- Through analysis of strong metric dimensions, the minimum number of monitoring points required for various subsection graphs may be determined exactly.
- By carefully placing the sensors, this optimization technique improved problem identification abilities while using less resources.

5.6|Use in Real Life and Importance

- Metric dimensions are essential for process monitoring, risk mitigation, and troubleshooting in the real chemical industry, as demonstrated by the practical application of these dimensions in chemical graph theory.
- Graph theory investigations could provide useful insights for placing sensors in a way that would improve operational resilience and efficiency.

5.7|Theoretical Perspectives for Improving Fault Diagnosis Techniques

- Metric dimension studies yield theoretical knowledge that is crucial to enhancing fault diagnostic methods and ensuring that these strategies are effective in addressing real-world operational problems.
- Understanding the topological nature of chemical graphs helps to improve operational safety and reliability by facilitating the development of improved defect identification tools.

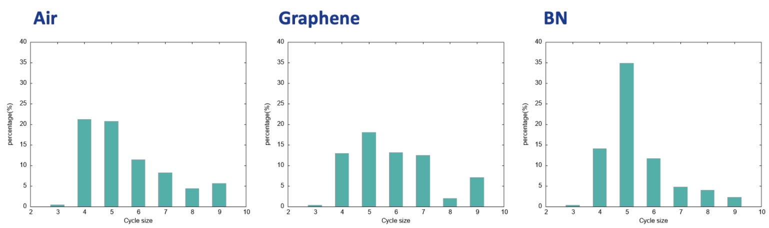

Figure 7. Size distribution of the water molecules' H-bonded rings and cycles in the condensed phase of 2D MolGraphs. The interfaces between air and water are on the left; graphene and water are on the middle; and BN and water are on the right.

To sum up, the incorporation of principles from graph theory, namely metric dimensions, into fault diagnostic procedures for chemical process facilities provides a methodical way to guarantee financial viability, safety, and efficiency. The chemical industry can greatly benefit from innovation and improved fault diagnosis techniques through the actual implementation of these theoretical findings.

6|Conclusion

The strong metric dimension is a useful notion with various applications in many fields, including networks security, robotics, wireless sensor networks, GPS navigation system, fault tolerance and network disruption. In this article, we extended the study of the strong metric dimension by finding the strong metric dimension of $HC(x, y, z)$ for $x = y = z \geq 2$ by establishing a relationship between covering number of strong resolving graph $HC(x, y, z)_{SR}$ and the strong metric dimension. We conclude that $sdim(HC(x, y, z)) = 3(x + y + z) - 12$. In future we extend our work by finding the strong metric dimension of hollow coronoid when x, y, z are not equal to each other and further by studying other invariant of metric dimension.

7|Future Recommendations

This paper presents an important advancement in studying the strong metric dimension of hollow coronoid structures. However, there are several promising directions for future work:

(1) Investigate the strong metric dimension of hollow coronoid structures where x, y, and z are not equal. This paper focused on the case where the three sides of the hollow coronoid structure are symmetric. Analyzing asymmetric hollow coronoids where $x \neq y \neq z$ would be an interesting extension.

(2) Explore other metric dimension invariants of hollow coronoids. In addition to the strong metric dimension, parameters like fractional metric dimension, mixed metric dimension, k-metric dimension etc. could provide further insights into these chemical structures when transformed into graphs.

(3) Examine other classes of chemical structures. The techniques used in this paper could be applied to find the strong metric dimension of other chemicals like benzenoids, phenylenes, polyhexes etc. This would expand our understanding of chemical graphs.

(4) Consider weighted graphs. Assigning weights to edges of the graph representation could reveal new findings regarding resolving sets and metric dimensions. The interplay between weights and shortest paths may impact the strong metric dimension.

(5) Develop computational methods and algorithms. Efficient methods to calculate the strong metric dimension for large chemical graphs would enable rapid analysis. Approximation algorithms and heuristics could produce useful results at scale.

(6) Explore applications of the strong metric dimension. This parameter has diverse applications in areas like robot navigation, network discovery, fault diagnosis etc. Relating the results to practical uses and implementations would demonstrate the utility of this research.

In summary, this work opens up many possibilities for further theoretical studies of metric dimensions of chemical structures, development of algorithms, and real-world applications. Building on these findings could uncover new insights at the intersection of graph theory, metric geometry and chemistry.

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