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Resolving Open Problems on the Hyper-Zagreb Index and its Chemical Applications

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Abstract: Topological indices are numerical invariants derived from molecular graphs and play an important role in characterizing chemical compounds and predicting their properties. Among the earliest descriptors are the classical Zagreb indices introduced by Gutman and Trinajstić in 1972. A more recent development is the hyper-Zagreb index (*HM*), defined as $HM(G)=\sum_{v_iv_j\in E(G)}(d_i+d_j)^2$, where d_i. denotes the degree of vertex v_i. In 2023, Hayat et al. posed an open problem concerning bounds on the *HM* index under fixed vertex-connectivity or edge-connectivity, along with the characterization of the corresponding extremal graphs. In this work, the problem is resolved by determining the extremal graphs that maximize *HM* index under these constraints. The investigation is further extended to several additional extremal problems, including graphs with a given number of leaves, chromatic number, and independence number. The associated extremal graphs are identified in each case. In addition, the chemical relevance of *HM* is examined through QSPR studies. Finally, the conclusion is presented.}

Keywords: Extremal graph, Hyper-Zagreb index, Vertex-connectivity, Edge-connectivity, QSPR analysis.
MSC: 05C90, 05C07, 05C35.

INTRODUCTION

MATHEMATICAL chemistry is a multidisciplinary area that employs mathematical tools to investigate chemical structures, reactions, and properties. In particular, researchers apply graph-theoretic methods to analyze molecular systems with enhanced accuracy and efficiency by modeling molecules as graphs where atoms serve as vertices and chemical bonds as edges.

Topological indices are a key concept in this approach. These numerical invariants are obtained from the molecular graph and capture essential structural characteristics such as symmetry and connectivity. These invariants are widely utilized in quantitative structure–property relationship (QSPR) studies to explain chemical properties by providing a compact mathematical representation of molecular structure. Through QSPR models, topological indices help to link molecular structure to experimental properties, aiding in drug design, materials discovery, and toxicity prediction.

Since Wiener's groundbreaking work in 1947,[1] many topological indices have been used in academic research to describe molecular structures using parameters like degree, eccentricity, and distance.[2–4] Degree-based descriptors have been especially important among these, having a significant impact on both theoretical research and real-world applications.[5,6] In 1972, Gutman and Trinajstić described the Zagreb indices,[7] which are among the earliest degree-based topological indices. For a graph G with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge set $E(G)$, the first Zagreb index (M_1) and the second Zagreb index (M_2) are formulated as follows:

$$M_1(G)=\sum_{v_iv_j\in E(G)}(d_i+d_j),\qquad M_2(G)=\sum_{v_iv_j\in E(G)}d_id_j,$$

where d_i represents the degree of the vertex v_i. These indices have been very helpful in analyzing different molecular properties, such as complexity, chirality, and hetero-systems. These indices have been the subject of a substantial body of literature that covers both mathematical and chemical aspects. For example, Liu and Gutman gave some bounds on the M_1 and M_2 indices for connected graphs.[8] Das and Gutman explored the M_2 index in the context of a graph and its complement.[9] Das compared the M_1 and M_2 indices.[10] Gutman et al. provided a comprehensive solution to the problem of finding the lowest value of M_1 among all graphs with a fixed number of pendant vertices.[11] Liu et al. described the maximal graphs for M_1 within a class of graphs characterized by a certain vertex-connectivity.[12] Over the past 30 years, Gutman and Das presented a comprehensive survey of the literature on M_1.[13] For further results on the M_1 and M_2 indices, the reader may consult the relevant references.[14–17]

Recently, Shirdel et al. presented the hyper-Zagreb index (HM),[18] which is a refinement of the first Zagreb index. The HM index is defined as

$$HM(G) = \sum_{v_i v_j \in E(G)} (d_i + d_j)^2.$$

Mirajkar et al. found that HM provides higher accuracy in modelling *DHVAP*, *HVAP*, entropy, and acentric factor of octanes.[19]

The effectiveness of the HM index in explaining some physicochemical properties of monocarboxylic acids was examined in the literature.[20]

Elumalai et al. provided new bounds for the HM index of connected graphs.[21–23] Liu and Tang established the maximum value of the HM index for trees, unicyclic graphs, and bicyclic graphs with a specified matching number, and further characterized the corresponding extremal graphs.[24] Raza et al. examined the extremal trees with respect to the HM index under constraints on maximum degree.[25] For further results on the HM index, the reader may consult the relevant references.[26,27] Hayat et al. posed some interesting open problems on HM,[20] as reported below:

- **Problem:** Determine sharp bounds for HM of graphs with specified vertex-connectivity or edge-connectivity, and classify extremal graphs.
- **Problem:** Find sharp bounds with respect to HM of graphs with prescribed diameter or matching number, and identify the extremal graphs.

In recent studies, maximal graphs with respect to HM for a fixed graph order and either a prescribed diameter or matching number were investigated.[28,29] In this paper, we classify graphs with the highest HM index by considering those with prescribed vertex-connectivity, edge-connectivity, number of leaves, chromatic number, or independence number. Furthermore, we analyze the contribution of the HM index to the modeling of structure–property relationships of nonane isomers.

MATHEMATICAL RESULTS ON *HM* OF GRAPHS

In this section, we explore the mathematical properties of HM for graphs.

Lemma 2.1. (*i*) *$HM(G) > HM(G-e)$ for any edge $e \in E(G)$, and* (*ii*) *$HM(G+e) > HM(G)$ for $e \notin E(G)$.*

The split graph $SP(n,\beta)$ is a graph of order n with independence number β, defined as

$$SP(n,\beta) = \overline{K_\beta} \vee K_{n-\beta}$$

where $\vee$ denotes the join of graphs and the overline indicates the graph complement. Applying Lemma 2.1, it is simple to observe the following result:

Theorem 2.2. *Let G be a graph of order n with independence number β. Then*

$$HM(G) \le 2(n-\beta)(n-\beta-1)(n-1)^2 + \beta(n-\beta)(2n-\beta-1)^2$$

with equality iff $G \cong SP(n,\beta)$.

The **Turán graph**, represented by $T(n,r)$, is a complete r-partite graph on n vertices. More specifically, the vertex set is divided into r disjoint independent parts such that the sizes of any two parts differ by at most one. That is, if the part sizes are n_1, n_2, ..., n_r, then

$$\sum_{i=1}^{r} n_i = n \quad \text{and} \quad |n_i - n_j| \le 1 \quad \text{for all } i, j.$$

Each vertex is directly connected to all vertices outside its own part. We write $K_{n_1, n_2, \ldots, n_r}$ to represent a complete r-partite graph with parts of sizes n_1, n_2, ..., n_r such that $n_1 \ge n_2 \ge \ldots \ge n_r$ We now describe the maximal graphs for HM within a class of graphs identified by a specific chromatic number.

Theorem 2.3. *Let G be a graph of order n with chromatic number r. Then*

$$\begin{aligned} HM(G) \le{} & t(r-t)\left\lfloor \frac{n}{r} \right\rfloor \left\lceil \frac{n}{r} \right\rceil \left(2n - \left\lceil \frac{n}{r} \right\rceil - \left\lfloor \frac{n}{r} \right\rfloor\right)^2 \\ & + 4\binom{r-t}{2} \left\lfloor \frac{n}{r} \right\rfloor^2 \left(n - \left\lfloor \frac{n}{r} \right\rfloor\right)^2 \qquad (1) \\ & + 4\binom{t}{2} \left\lceil \frac{n}{r} \right\rceil^2 \left(n - \left\lceil \frac{n}{r} \right\rceil\right)^2, \end{aligned}$$

where $n = r\left\lfloor \frac{n}{r} \right\rfloor + t$, $0 \le t < r$. Furthermore, the equality occurs in Eq.(1) iff $G \cong T(n,r)$.

Proof. Since G has a graph of order n with chromatic number r, G can be partitioned into r independent sets of sizes n_1, n_2, ..., n_r. Without loss of generality, suppose $n_1 \ge n_2 \ge \ldots \ge n_r \ge 1$. According to Lemma 2.1., we say that $HM(G) \le HM(K_{n_1,n_2,\ldots,n_r})$ with equality iff $G \cong K_{n_1,n_2,\ldots,n_r}$. If $n_1 - n_r \le 1$, then $G \cong T(n,r)$ and so the equality occurs in Eq.(1). Otherwise, $n_1 - n_r \ge 2$. For $r = 2$, we obtain

$$\begin{aligned}HM(K_{n_1-1,n_2+1}) - HM(K_{n_1,n_2}) &= (n_1-1)(n_2+1)(2n-n_1-n_2)^2\\ &\quad - n_1 n_2(2n-n_1-n_2)^2\\ &= (n_1-n_r-1)n^2 > 0\end{aligned}$$

as $n_1 + n_2 = n$. For $r \ge 3$, one can easily see that

$$\begin{aligned}&HM(K_{n_1-1,n_2,\ldots,n_r+1}) - HM(K_{n_1,n_2,\ldots,n_r})\\
&= (n_1-1)(n_r+1)(2n-n_1-n_r)^2 - n_1 n_r(2n-n_1-n_r)^2\\
&+ (n_1-1)\sum_{i=2}^{r-1} n_i(2n-n_1-n_i+1)^2 - n_1\sum_{i=2}^{r-1} n_i(2n-n_1-n_i)^2\\
&+ (n_r+1)\sum_{i=2}^{r-1} n_i(2n-n_r-n_i-1)^2 - n_r\sum_{i=2}^{r-1} n_i(2n-n_r-n_i)^2\\
&= (n_1-n_r-1)(2n-n_1-n_r)^2 - \sum_{i=2}^{r-1} n_i(2n-n_1-n_i+1)^2\\
&+ \sum_{i=2}^{r-1} n_i(2n-n_r-n_i-1)^2\\
&+ n_1\sum_{i=2}^{r-1} n_i((2n-n_1-n_i+1)^2-(2n-n_1-n_i)^2)\\
&- n_r\sum_{i=2}^{r-1} n_i((2n-n_r-n_i)^2-(2n-n_r-n_i-1)^2)\\
&= (n_1-n_r-1)(2n-n_1-n_r)^2\\
&+ \sum_{i=2}^{r-1} n_i((2n-n_r-n_i-1)^2-(2n-n_1-n_i+1)^2)\\
&+ n_1\sum_{i=2}^{r-1} n_i(2(2n-n_1-n_i)+1) - n_r\sum_{i=2}^{r-1} n_i(2(2n-n_r-n_i)-1)\\
&> \sum_{i=2}^{r-1} n_i(2n_1(2n-n_1-n_i)-2n_r(2n-n_r-n_i)) + \sum_{i=2}^{r-1} n_i(n_1-n_r)\\
&> 2\sum_{i=2}^{r-1} n_i(n_1-n_r)(2n-n_i-n_1-n_r) \ge 0.\end{aligned}$$

Thus we have $HM(K_{n_1-1,n_2,\ldots,n_r+1}) > HM(K_{n_1,n_2,\ldots,n_r})$. From this result, we obtain the following:

$$HM(K_{n_1,n_2,\ldots,n_r}) < HM(K_{n_1-1,n_2,\ldots,n_r+1}) < \cdots < HM(T(n,r)).$$

The inequality in Eq.(1) holds strictly. Thus, the theorem is proved. ■

Let $S(n_1,n_2,\ldots,n_{n-p})$ be a graph with n vertices, consisting of a clique K_{n-p} with $n-p$ vertices and p leaves, where each n_i represents the number of leaves attached to the i-th vertex of the clique K_{n-p} and $\sum_{i=1}^{n-p} n_i = p$ with $n_i \ge 0$ for $1 \le i \le n-p$. A special case of this graph is when all $n_i = 0$, i.e., no leaves are attached. In this case, the graph is simply the complete graph K_n, and we write: $S(0,0,\ldots,0) \cong K_n$. The pineapple graph $K_{n,p}$ is a graph obtained by identifying one vertex of K_{n-p} with central vertex of star $K_{1,p}$, that is, $K_{n,p} \cong S(p,\underbrace{0,\ldots,0}_{n-p-1})$. One can easily see that

$$\begin{aligned}HM(K_{n,p}) &= (n-p-1)(2n-p-2)^2\\ &\quad + 4\binom{n-p-1}{2}(n-p-1)^2 + pn^2.\end{aligned}$$

We now present an upper bound on $HM(G)$ of graph G in terms of n and the number of leaves p, and identify the maximal graphs.

Theorem 2.4. Let G be a graph of order n with $p(\le n-2)$ leaves. Then

$$\begin{aligned}HM(G) &\le (n-p-1)(2n-p-2)^2\\ &\quad + 4\binom{n-p-1}{2}(n-p-1)^2 + pn^2\end{aligned} \tag{2}$$

with equality iff $G \cong K_{n,p}$. ■

Proof. If $p = 0$, then from Lemma 2.1., it is obvious that $HM(G) \le HM(K_n) = 2n(n-1)^3$ with equality iff $G \cong K_n$. Otherwise, $p \ge 1$. Let H be a graph with n vertices and the number of leaves $p(\ge 1)$ such that the hyper-Zagreb index $HM(H)$ is maximum. So $HM(G) \le HM(H)$ with equality iff $G \cong H$. Let $q = n-p$. Then we have $q \ge 2$. We take a set of leaves $S \subseteq V(H)$ with $|S| = p$. By Lemma 2.1., we obtain $H[V(H)-S] \cong K_{n-p}$. Thus the graph H has the form $H \cong S(n_1,n_2,\ldots,n_{n-p})$. If $n_1 = p$, then $n_2 = n_3 = \cdots = n_{n-p} = 0$ and hence

$$\begin{aligned}HM(G) \le HM(H) &= HM(S(n_1,n_2,\ldots,n_{n-p})) = HM(K_{n,p})\\ &= (n-p-1)(2n-p-2)^2\\ &\quad + 4\binom{n-p-1}{2}(n-p-1)^2 + pn^2\end{aligned}$$

with equality iff $G \cong K_{n,p}$. Otherwise, $n_1 < p$. Thus we have $n_2 \ge 1$. Without loss of generality, we suppose that there is a positive integer $t(\ge 2)$ with $n_t \ge 1$ and $n_{t+1} = n_{t+2} = \cdots = n_{n-p} = 0$.

Claim 1.

$$\begin{aligned}&HM(S(n_1+1,n_2,\ldots,n_t-1,\ldots,n_{n-p}))\\ &> HM(S(n_1,n_2,\ldots,n_t,\ldots,n_{n-p})).\end{aligned}$$

Proof of Claim 1. Now,

$$\begin{aligned}&HM(S(n_1+1,n_2,\ldots,n_t-1,\ldots,n_{n-p}))\\
&-HM(S(n_1,n_2,\ldots,n_t,\ldots,n_{n-p})) = (n_1+1)(n+n_1-p+1)^2\\
&-n_1(n+n_1-p)^2 + (n_t-1)(n+n_t-p-1)^2 - n_t(n+n_t-p)^2\\
&+\sum_{\substack{i=2\\ i\ne t}}^{n-p}((2n-2p+n_1+n_i-1)^2-(2n-2p+n_1+n_i-2)^2)\\
&+\sum_{\substack{i=2\\ i\ne t}}^{n-p}((2n-2p+n_t+n_i-3)^2-(2n-2p+n_t+n_i-2)^2)\end{aligned}$$

$$
\begin{aligned}
&= ((n+n_1-p+1)^2-(n+n_1-p)^2)n_1\\
&+((n+n_t-p-1)^2-(n+n_t-p)^2)(n_t-1)\\
&+(n+n_1-p+1)^2-(n+n_t-p)^2\\
&+\sum_{\substack{i=2\\ i\neq t}}^{n-p}(2(2n-2p+n_1+n_i-2)+1)\\
&-\sum_{\substack{i=2\\ i\neq t}}^{n-p}(2(2n-2p+n_t+n_i-2)-1)\\
&=(2n+2n_1-2p+1)n_1-(2n+2n_t-2p-1)(n_t-1)\\
&+(2n+2n_1-2p+1)+2\sum_{\substack{i=2\\ i\neq t}}^{n-p}(n_1-n_t+1)>0
\end{aligned}
$$

as $n-p\geq 2$. Thus, the **Claim 1.** is proved.

By applying **Claim 1.** repeatedly, we get the following inequalities:

$$
\begin{aligned}
&HM(S(n_1,n_2,\ldots,n_t,\ldots,n_{n-p}))\\
&< HM(S(n_1+1,n_2,\ldots,n_t-1,\ldots,n_{n-p}))\\
&<\cdots< HM(S(p-1,1,\underbrace{0,\ldots,0}_{n-p-2}))\\
&< HM(S(p,\underbrace{0,\ldots,0}_{n-p-1}))=HM(K_{n,p}).
\end{aligned}
$$

Using the above result, we obtain

$$HM(G)\leq HM(H)=HM(S(n_1,n_2,\ldots,n_{n-p}))<HM(K_{n,p}).$$

The result in Eq.(2) holds strictly. Thus, the theorem is proved. ■

We now prove that for a graph G with n vertices and vertex connectivity k, the graph $(K_1\cup K_{n-k-1})\vee K_k$ maximizes the value $HM(G)$.

Theorem 2.5. *Let G be a graph of order n with vertex connectivity k. Then*

$$
\begin{aligned}
HM(G)\leq{}& 4\binom{k}{2}(n-1)^2+4\binom{n-k-1}{2}(n-2)^2\\
&+k(n-k-1)(2n-3)^2+k(n+k-1)^2
\end{aligned}
\tag{3}
$$

with equality iff $G\cong(K_1\cup K_{n-k-1})\vee K_k$.

Proof. Let H be a graph of order n and vertex connectivity k such that the hyper-Zagreb index $HM(H)$ is maximum. So $HM(G)\leq HM(H)$ with equality iff $G\cong H$. Consider a vertex cut $S\subseteq V(H)$ with $|S|=k$, for which the removal of S disconnects the graph H. Since H maximizes the hyper-Zagreb index $HM(H)$ among all such graphs of order n with vertex connectivity k, it follows that H–S must have exactly two connected components. Denote these components by H_1 and H_2, with $|V(H_1)|=k_1$ and $|V(H_2)|=n-k-k_1$. Without loss of generality, we suppose that $k_1\leq n-k-k_1$, that is, $1\leq k_1\leq\lfloor\frac{n-k}{2}\rfloor$ (H_1 is the smaller of the two components). By Lemma 2.1., we can state that $H_1\cong K_{k_1}$, $H[S]\cong K_k$, $H_2\cong K_{n-k-k_1}$ and each vertex in S is directly connected to all the vertices in $H_1\cup H_2$. Thus, the graph H has the structure $H\cong K_k\vee(K_{k_1}\cup K_{n-k-k_1})$, where $\vee$ denotes the join of graphs. This structure ensures maximal connectivity and pairwise proximity, thereby maximizing the hyper-Zagreb index. If $k_1=1$, then we have $H\cong(K_1\cup K_{n-k-1})\vee K_k$ and hence

$$
\begin{aligned}
HM(G)&\leq HM(H)=HM(K_k\vee(K_1\cup K_{n-k-1}))\\
&=4\binom{k}{2}(n-1)^2+4\binom{n-k-1}{2}(n-2)^2\\
&+k(n-k-1)(2n-3)^2+k(n+k-1)^2
\end{aligned}
$$

with equality iff $G\cong(K_1\cup K_{n-k-1})\vee K_k$. The result holds in Eq(3).

Otherwise, $2\leq k_1\leq\lfloor\frac{n-k}{2}\rfloor$. One can easily see that the degree d_i of vertex v_i is given by:

$$
d_i=\begin{cases}
n-1 & \text{for } v_i\in S,\\
k_1+k-1 & \text{for } v_i\in V(H_1),\\
n-k_1-1 & \text{for } v_i\in V(H_2).
\end{cases}
$$

Let $k_2=n-k-k_1$. Then $k_2\geq k_1$. We have $HM(G)\leq HM(H)=HM((K_{k_1}\cup K_{k_2})\vee K_k)$. We now prove the following claim.

Claim 2.

$$HM((K_{k_1-1}\cup K_{k_2+1})\vee K_k)>HM((K_{k_1}\cup K_{k_2})\vee K_k).$$

Proof of Claim 2. Now,

$$
\begin{aligned}
&HM((K_{k_1-1}\cup K_{k_2+1})\vee K_k)\\
&-HM((K_{k_1}\cup K_{k_2})\vee K_k)=4\binom{k_1-1}{2}(k+k_1-2)^2\\
&+4\binom{k_2+1}{2}(k+k_2)^2+k(k_1-1)(2n-k_2-3)^2\\
&+k(k_2+1)(2n-k_1-1)^2-4\binom{k_1}{2}(k+k_1-1)^2\\
&-4\binom{k_2}{2}(k+k_2-1)^2-kk_1(2n-k_2-2)^2\\
&-kk_2(2n-k_1-2)^2\\
&=2(k_1-1)[(k_1-2)(k+k_1-2)^2-k_1(k+k_1-1)^2]\\
&+2k_2[(k_2+1)(k+k_2)^2-(k_2-1)(k+k_2-1)^2]\\
&+k[(k_1-1)(2n-k_2-3)^2-k_1(2n-k_2-2)^2]\\
&+k[(k_2+1)(2n-k_1-1)^2-k_2(2n-k_1-2)^2]\\
&=2(k_1-1)[-2(k+k_1-2)^2-k_1(2k+2k_1-3)]\\
&+2k_2[2(k+k_2)^2+(k_2-1)(2k+2k_2-1)]\\
&+k[-(2n-k_2-3)^2-k_1(4n-2k_2-5)\\
&+(2n-k_1-1)^2+k_2(4n-2k_1-3)].
\end{aligned}
\tag{4}
$$

Since $k_2 \geq k_1$, we obtain

$$(2n - k_1 - 1)^2 > (2n - k_2 - 3)^2, \text{ and}$$
$$k_2(4n - 2k_1 - 3) > k_1(4n - 2k_2 - 5).$$

Thus we have

$$-(2n - k_2 - 3)^2 - k_1(4n - 2k_2 - 5)$$
$$+(2n - k_1 - 1)^2 + k_2(4n - 2k_1 - 3) > 0.$$

Applying the above result in Eq(4), we get

$$\begin{aligned}&HM((K_{k_1-1} \cup K_{k_2+1}) \vee K_k) - HM((K_{k_1} \cup K_{k_2}) \vee K_k)\\&> 2(k_1 - 1)[-2(k + k_1 - 2)^2 - k_1(2k + 2k_1 - 3)]\\&+ 2k_2[2(k + k_2)^2 + (k_2 - 1)(2k + 2k_2 - 1)]\\&> 2(k_1 - 1)[-2(k + k_1 - 2)^2 - k_1(2k + 2k_1 - 3\\&+ 2(k + k_2)^2 + (k_2 - 1)(2k + 2k_2 - 1)].\end{aligned} \tag{5}$$

If $k_2 \geq k_1 + 1$, then

$$(k + k_2)^2 > (k + k_1 - 2)^2,$$
$$(k_2 - 1)(2k + 2k_2 - 1) > k_1(2k + 2k_1 - 3),$$

and hence

$$-2(k + k_1 - 2)^2 - k_1(2k + 2k_1 - 3)$$
$$+2(k + k_2)^2 + (k_2 - 1)(2k + 2k_2 - 1) > 0.$$

Using the above result, we obtain

$$HM((K_{k_1-1} \cup K_{k_2+1}) \vee K_k) > HM((K_{k_1} \cup K_{k_2}) \vee K_k).$$

Otherwise, $k_2 = k_1$. From Eq(5), we obtain

$$\begin{aligned}&HM((K_{k_1-1} \cup K_{k_2+1}) \vee K_k) - HM((K_{k_1} \cup K_{k_2}) \vee K_k)\\&> 2(k_1 - 1)[-2(k + k_1 - 2)^2 - k_1(2k + 2k_1 - 3\\&+2(k + k_1)^2 + (k_1 - 1)(2k + 2k_1 - 1)]\\&= 2(k_1 - 1)(6k + 8k_1 - 7) > 0.\end{aligned}$$

Hence $HM((K_{k_1-1} \cup K_{k_2+1}) \vee K_k) > HM((K_{k_1} \cup K_{k_2}) \vee K_k)$. Thus, the **Claim 2.** is proved.

By employing the **Claim 2.** several times, we get

$$HM((K_{k_1} \cup K_{k_2}) \vee K_k) < HM((K_{k_1-1} \cup K_{k_2+1}) \vee K_k) < \cdots$$
$$< HM((K_1 \cup K_{n-k-1}) \vee K_k).$$

Utilizing the above result, we get

$$HM(G) \leq HM((K_{k_1} \cup K_{k_2}) \vee K_k) < HM((K_1 \cup K_{n-k-1}) \vee K_k).$$

Thus, the theorem is proved. ■

Theorem 2.6. Let G be a graph of order n with edge connectivity k'. Then

$$\begin{aligned}HM(G) \leq\ & 4\binom{k'}{2}(n-1)^2 + 4\binom{n-k'-1}{2}(n-2)^2\\&+k'(n - k' - 1)(2n - 3)^2 + k'(n + k' - 1)^2\end{aligned} \tag{6}$$

with equality iff $G \cong (K_1 \cup K_{n-k'-1}) \vee K_{k'}$.

Proof. We consider a function

$$\begin{aligned}h(y) =\ & 4\binom{y}{2}(n-1)^2 + 4\binom{n-y-1}{2}(n-2)^2\\&+ y(n - y - 1)(2n - 3)^2 + y(n + y - 1)^2\\&= 2y(y - 1)(n - 1)^2 + 2(n - y - 1)(n - y - 2)(n - 2)^2\\&+ y(n - y - 1)(2n - 3)^2 + y(n + y - 1)^2,\ y \leq k'.\end{aligned}$$

Then

$$\begin{aligned}h'(y) =\ & 2(y - 1)(n - 1)^2 + 2y(n - 1)^2\\&-2(n - y - 2)(n - 2)^2 - 2(n - y - 1)(n - 2)^2\\&+(n - y - 1)(2n - 3)^2 - y(2n - 3)^2\\&+(n + y - 1)^2 + 2y(n + y - 1)\\&= 2(2y - 1)[(n - 1)^2 - (n - 1.5)^2]\\&+2(n - y - 1)[(n - 1.5)^2 - (n - 2)^2]\\&+2(n - y - 2)[(n - 1.5)^2 - (n - 2)^2]\\&+(n + y - 1)^2 + 2y(n + y - 1) > 0.\end{aligned}$$

So $h(y)$ is an increasing function on $y \leq k'$, and therefore $h(k) \leq h(k')$ as $k \leq k'$ (where k is vertex connectivity). By **Theorem 2.5.**, we get the result Eq(6). Furthermore, the equality occurs iff $G \cong (K_1 \cup K_{n-k'-1}) \vee K_{k'}$. ■

CHEMICAL APPLICATIONS OF THE *HM* INDEX

Topological indices are based on mathematical chemistry, so it is crucial to evaluate their chemical relevance in addition to their theoretical aspects. Researchers discovered that *HM* strongly explains different physicochemical properties, including those of octanes, monocarboxylic acids, and the boiling point of benzenoid hydrocarbons.[19,20,30]

Recent studies have explored the chemical applications of topological indices.[31–33]

Building upon these findings, this section examines the chemical applicability of *HM* by constructing linear, quadratic, and cubic regression models for standard enthalpy of vaporization (*DHVAP*) of nonane isomers (all C_9H_{20}). Table 1 presents the theoretical *HM* values along with the *DHVAP* for nonane isomers. The experimental *DHVAP* values were collected from the literature.[34] Since all nonane isomers have identical molecular size (n = 9, m = 8), the observed structure–property relationships reflected genuine molecular structural information rather than size effects. To analyze the predictive ability of the *HM* index, we use the following regression relations:

$$Y = \ell_1 X + \ell_2, \tag{7}$$

$$Y = m_1 X^2 + m_2 X + m_3, \tag{8}$$

$$Y = n_1 X^3 + n_2 X^2 + n_3 X + n_4, \tag{9}$$

where Y, X represent property and descriptor, respectively, and ℓ_1, ℓ_2, m_1, m_2, m_3, n_1, n_2, n_3, and n_4 are fitting parameters. Along with relations Eq(7), Eq(8), and Eq(9), we also take into account some other statistical parameters such as the coefficient of determination (R^2), *F*-test (*F*), root mean square error (*RMSE*), and significance F(*SF*) to better understand the regression relationships.

For *DHVAP*, the Eq(7) takes the following form:

$$\begin{aligned} &DHVAP = -0.0473(HM) + 50.7080, \\ &R^2 = 0.7045, \qquad RMSE = 0.8563, \\ &F = 78.6630, \qquad SF = 2.99 \times 10^{-10}. \end{aligned} \tag{10}$$

Similarly, the Eq(8) takes the following form:

$$\begin{aligned} &DHVAP = 0.000228(HM^2) - 0.1260(HM) + 57.3117, \\ &R^2 = 0.7227, \qquad RMSE = 0.8296, \\ &F = 41.6912, \qquad SF = 1.23 \times 10^{-09}. \end{aligned} \tag{11}$$

Finally, the Eq(9) takes the following form:

$$\begin{aligned} &DHVAP = -4.42 \times 10^{-06}(HM^3) + 0.002544(HM^2) \\ &\qquad -0.5218(HM) + 79.3692, \\ &R^2 = 0.731, \qquad RMSE = 0.8170, \\ &F = 28.0775, \qquad SF = 5.71 \times 10^{-09}. \end{aligned} \tag{12}$$

Table 1. Theoretical HM and experimental DHVAP for nonane isomers.

Nonanes	*HM*	*DHVAP*	Nonanes	HM	DHAVP
C9:1	114	46.44	C9:19	192	42.23
C9:2	130	44.65	C9:20	170	42.93
C9:3	132	44.75	C9:21	166	41.42
C9:4	132	44.75	C9:22	188	40.84
C9:5	168	42.28	C9:23	194	42.28
C9:6	150	43.79	C9:24	152	43.84
C9:7	148	42.87	C9:25	150	42.98
C9:8	148	42.87	C9:26	176	43.04
C9:9	146	42.82	C9:27	154	43.95
C9:10	172	42.66	C9:28	234	41
C9:11	152	43.84	C9:29	208	41
C9:12	150	42.98	C9:30	222	38.1
C9:13	172	42.66	C9:31	212	41.75
C9:14	134	44.81	C9:32	192	42.02
C9:15	134	44.81	C9:33	196	42.55
C9:16	190	41.91	C9:34	170	42.93
C9:17	186	40.57	C9:35	180	43.36
C9:18	184	40.17			

Figure 1. shows the linear fit for model Eq(10), Figure 2. displays the quadratic fit for model Eq(11), and Figure 3. shows the cubic fit for model Eq(12). The blue, purple, and orange lines indicate the best-fit lines corresponding to the linear, quadratic, and cubic models, respectively, and the green circles indicate the ordered pairs (x, y), where x and y are the *HM* index and *DHVAP* of nonane isomers, respectively.

To evaluate the performance of the *HM* index in different regression models, we analyze relations Eqs(10–12) and Figures 1–3. Based on the linear model Eq(10), the *HM* index accounts for 70 % of the variance in *DHVAP*, as visualized in Figure 1. The quadratic model Eq(11) shows that *HM* explains 72 % of the variance in *DHVAP*, as illustrated in Figure 2. Moreover, the cubic model Eq(12) indicates that *HM* explains 73 % of the variance in *DHVAP*, as visualized in Figure 3. The corresponding *SF* values are much smaller than 0.05, confirming the statistical significance of the models. Collectively, these results demonstrate that *HM* effectively models *DHVAP* for nonane isomers, with the observed structure–property relationships reflecting genuine structural information rather than size effects due to their identical molecular size (n = 9, m = 8).

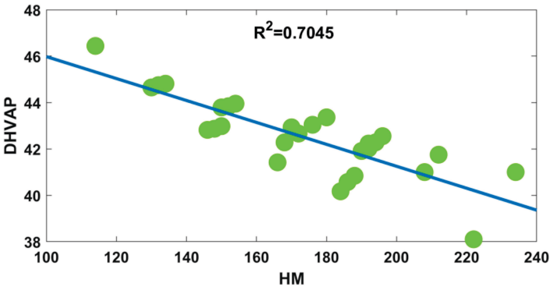

Figure 1. Linear fitting of *HM* with *DHVAP* for nonane isomers.

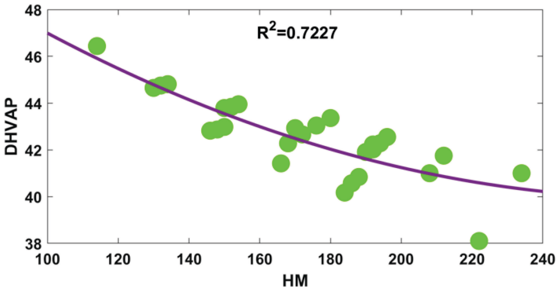

Figure 2. Quadratic fitting of *HM* with *DHVAP* for nonane isomers.

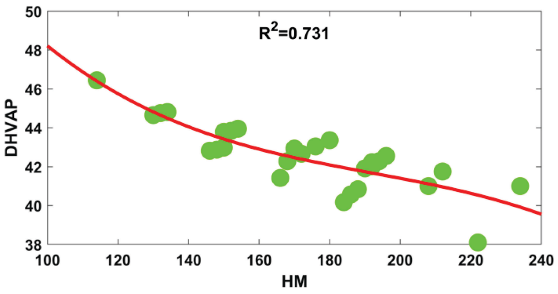

Figure 3. Cubic fitting of *HM* with *DHVAP* for nonane isomers.

Table 2. Definitions and references of degree-based topological indices used in this study.

Index	Definition	Ref.
M_1 (first Zagreb)	$\sum_{v_iv_j \in E(G)} (d_i + d_j)$	[7]
M_2 (second Zagreb)	$\sum_{v_iv_j \in E(G)} d_i d_j$	[7]
ALB (Albertson)	$\sum_{v_iv_j \in E(G)} \lvert d_i - d_j \rvert$	[36]
RM_2 (modified second Zagreb)	$\sum_{v_iv_j \in E(G)} \frac{1}{d_i d_j}$	[37]
PL (Platt)	$\sum_{v_iv_j \in E(G)} (d_i + d_j - 2)$	[38,39]
F (forgotten)	$\sum_{v_iv_j \in E(G)} (d_i^2 + d_j^2)$	[40]
ISI (inverse sum indeg)	$\sum_{v_iv_j \in E(G)} \frac{d_i d_j}{d_i + d_j}$	[41,42]
HM (hyper-Zagreb)	$\sum_{v_iv_j \in E(G)} (d_i + d_j)^2$	[18]

DEGENERACY

Topological indices are essential for establishing structure-property relationships as well as for distinguishing isomers. The ability of a topological index to discriminate between isomers is crucial for the encoding and computational processing of chemical structures.

Konstantinova introduced sensitivity (*ST*) to measure discriminative capability using the definition:

$$S_A = \frac{N - N_A}{N}, \tag{13}$$

where N and N_A represent the total number of isomers and the total number of isomers that the index A cannot differentiate, respectively.[35] An S_A value closer to 1 indicates a higher discriminative power of the index.

In this investigation, we evaluate the discriminative capabilities of the *HM* index alongside several established degree-based topological indices using octane isomers. Table 2. lists the definitions and references for all considered indices.

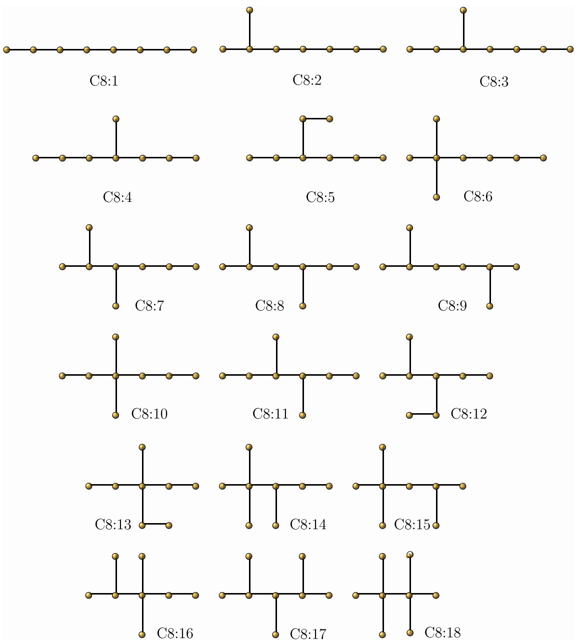

Figure 4. Molecular graphs of octane isomers.

Table 3. presents the calculated values of these indices for all octane isomers, and Figure 4. illustrates their molecular graphs.

Figure 5. illustrates the discriminative sensitivity values calculated using Konstantinova's formula. The *HM* index exhibits the highest sensitivity among all indices considered, with a value of 0.833. Indices such as M_2, RM_2, and *ISI* show moderately lower values (0.722), while M_1, *PL*, *F*, and *ALB* exhibit substantially lower discriminative power (0.333–0.444). These observations indicate that the *HM* index possesses strong structural discrimination capability and performs favorably compared with the other indices considered for distinguishing between isomeric molecular structures in QSPR studies.

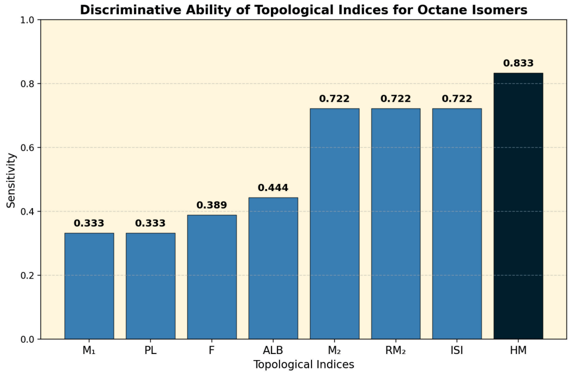

Figure 5. Discriminative ability of topological indices for octanes.

Table 3. The topological indices (*HM*, RM_2, M_1, M_2, *F*, *PL*, *ALB*, *ISI*) values for octanes.

Octanes	*HM*	RM_2	M_1	M_2	*F*	*PL*	*ALB*	*ISI*
C8:1	98	2.25	26	24	50	12	2	6.3333
C8:2	114	2.0833	28	26	62	14	6	6.3667
C8:3	116	2.1667	28	27	62	14	6	6.4833
C8:4	116	2.1667	28	27	62	14	6	6.4833
C8:5	118	2.25	28	28	62	14	6	6.6
C8:6	152	1.875	32	30	92	18	12	6.4
C8:7	134	2.0278	30	30	74	16	8	6.6167
C8:8	132	2	30	29	74	16	10	6.5167
C8:9	130	1.9167	30	28	74	16	10	6.4
C8:10	156	2	32	32	92	18	12	6.6
C8:11	136	2.1111	30	31	74	16	8	6.7333
C8:12	136	2.1111	30	31	74	16	8	6.7333
C8:13	160	2.125	32	34	92	18	12	6.8
C8:14	174	1.8333	34	35	104	20	14	6.7310
C8:15	168	1.7083	34	32	104	20	16	6.4333
C8:16	176	1.875	34	36	104	20	14	6.8143
C8:17	152	1.8889	32	33	86	18	10	6.75
C8:18	214	1.5625	38	40	134	24	18	6.8

CONCLUSIONS

In this paper, we analyzed the maximal graphs for *HM* among all connected graphs, under constraints on the graph order along with a specified vertex-connectivity or edge-connectivity. These problems were previously addressed as open challenges in the literature.[20] However, determining the minimum *HM* index and characterizing the minimal graphs among connected graphs with fixed order and given vertex or edge connectivity remain open problems. We also investigated graphs with a specified number of leaves, chromatic number, or independence number that maximize *HM*. Furthermore, the applicability of *HM* was investigated through the analysis of its structure–property relationships. We observed that *HM* effectively predicts the *DHVAP* of nonane isomers through linear, quadratic, and cubic regression models. Additionally, the discriminative power of *HM* compares favorably with several established degree-based indices when applied to octane isomers.

Future research may focus on establishing the lower bounds of *HM* for graphs with specified vertex-connectivity or edge-connectivity, as well as identifying the graphs that attain these extremal values.

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