Topological indices: the modified Schultz index

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Introduction

Chemical Graph Theory

interdisciplinary science that applies Graph Theory to the study of molecular structures. The molecules or chemical compounds are modeled by an undirected graph - the **molecular graph**:

vertices $\longrightarrow$ atoms or group of atoms

edges $\longrightarrow$ chemical bonds between atoms or group of atoms

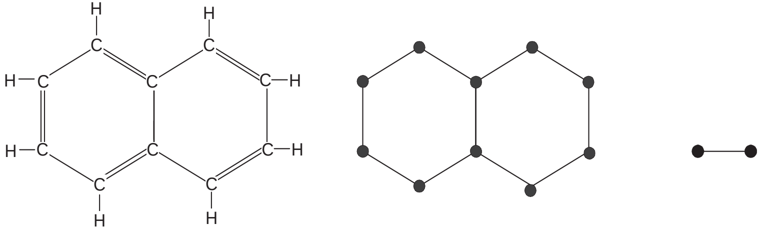


Figure: Structural formula and (hydrogen-supressed) molecular graphs of naphtalene, $C_{10}H_8$.

Topological indices

A **topological index** is a numerical parameter mathematically derived from the graph structure. It is a graph invariant thus it does not depend on the labeling or pictorial representation of the graph.

The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity (e.g., pharmacology).

The Wiener index

The **Wiener index** of a graph $G = (V, E)$

$$W(G) = \sum_{\{u,v\} \subset V} dist(u, v)$$

is the oldest topological index and its mathematical properties and chemical applications have been extensively studied.

The Wiener index was introduced by the chemist Harold Wiener (1947) for explaining the correlations between the boiling points of paraffins and the structure of their molecules:

$$t \approx aW + bp + c,$$

where t is the boiling point, W is the Wiener index, p is the polarity number and a, b and c are constants related to the isomeric group.

Other topological indices:

hyper-Wiener (Randić, 1993)	$WW(G) = \sum_{\{u,v\}\subset V} (d(u,v) + d^2(u,v))$
edge-Wiener (Dankelmann et al., 2009)	$W_e(G) = \sum_{\{e,f\}\subset E} d(e,f)$, where $e = e_1 e_2$, $f = f_1 f_2$, $d(e,f) = \min_{1\leq i,j\leq 2} d(e_i, f_j)$
1st Zagreb (Gutman et al., 1972)	$Z_1(G) = \sum_{u\in V} d^2(u)$
2nd Zagreb (Gutman et al., 1972)	$Z_2(G) = \sum_{uv\in E} d(u)d(v)$
Randić (Randić, 1975)	$R(G) = \sum_{uv\in E} (d(u)d(v))^{-1/2}$
Schultz (Schultz, 1989)	$S(G) = \sum_{\{u,v\}\subset V} (d(u) + d(v))d(u,v)$
modified Schultz (Gutman, 1994)	$S^*(G) = \sum_{\{u,v\}\subset V} d(u)d(v)d(u,v)$
Szeged (Gutman, 1994b)	$Sz(G) = \sum_{e=uv\in E} n_u(e)n_v(e)$, where $n_u(e) = \lvert\{w \in V : \ d(w,u) < d(w,v)\}\rvert$
Hosoya (Hosoya, 1971)	$Z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G,k)$, where $m(G,k)$ is the no. of k-matchings

Notation: $d(u,v) := dist(u,v)$ and $d(u)$ is the degree of vertex u.

The modified Schultz index

The **Schultz index**,

$$S(G) = \sum_{\{u,v\} \subset V} (d(u) + d(v)) dist(u, v)$$

was introduced by H. P. Schultz (1989).
For trees, the Schultz index is closely related to the Wiener index: if T is a tree on n vertices then (Klein et al., 1992)

$$S(T) = 4W(T) - n(n-1).$$

Motivated by the results on the Schultz index, Gutman (1994) introduced the **modified Schultz index**,

$$S^*(T) = \sum_{\{u,v\} \subset V} d(u)d(v) dist(u, v),$$

(also known as Gutman index) and presented an analogous relation with the Wiener index, in the case of trees (Gutman, 1994):

$$S^*(T) = 4W(T) - (n-1)(2n-1).$$

The modified Schultz index

From the above definitions it is immediate that

1. If $\delta(G)$ and $\Delta(G)$ are the minimum and maximum degree, respectively, of the vertices of G, then

$$2\delta(G)W(G) \leq S(G) \leq 2\Delta(G)W(G)$$

and

$$\delta^2(G)W(G) \leq S^*(G) \leq \Delta^2(G)W(G).$$

2. If G is p-regular then

$$S(G) = 2pW(G) \text{ and } S^*(G) = p^2W(G).$$

The modified Schultz index

The modified Schultz index of some graphs:

1. $S^*(C_n) = S(C_n) = 4W(C_n) = \begin{cases} \frac{n^3}{2}, & \text{if } n \text{ is even,} \\ \frac{n^3-n}{2}, & \text{if } n \text{ is odd.} \end{cases}$
2. $S^*(K_n) = (n-1)^2\binom{n}{2}$.
3. $S^*(P_n) = \frac{1}{3}(n-1)(2n^2-4n+3)$.
4. $S^*(K_{p,q}) = 2pq\left(\binom{p}{2}+\binom{q}{2}\right)+(pq)^2$.

Graph Operations

Definition

The **cartesian product** $G_1 \times G_2$ of graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, with $V_1 \cap V_2 = \emptyset$, is the graph with vertex set $V_1 \times V_2$ and two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ being adjacent whenever ($u_1 = v_1$ and $u_2 v_2 \in E_2$) or ($u_1 v_1 \in E_1$ and $u_2 = v_2$).

Proposition

Let $G_i = (V_i, E_i)$ be a graph of order n_i and dimension m_i, $i = 1, 2$. The modified Schultz index of the cartesian product $G_1 \times G_2$ is given by

$$\begin{aligned} S^*(G_1 \times G_2) &= \frac{1}{2} n_1(n_1+1) S^*(G_2) + \frac{1}{2} n_2(n_2+1) S^*(G_1) \\ &+ 2 m_2 n_2 S(G_1) + 2 m_1 n_1 S(G_2) \\ &+ \Big(Z_1(G_2) + Z_2(G_2) \Big) W(G_1) \\ &+ \Big(Z_1(G_1) + Z_2(G_1) \Big) W(G_2). \end{aligned}$$

Example

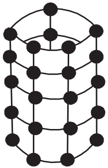


Figure: C_4-nanotube $G = P_5 x C_5$ with $S^*(G) = 8150$

The molecular graph of a C_4-nanotube is the cartesian product $P_m \times C_n$. For $m = n$ (n odd) we have

$$\begin{aligned}
\mathbf{S^*(P_m \times C_n)} &= \frac{1}{2}n(n+1)(S^*(P_n) + S^*(C_n)) \\
&+ 2n^2 S(P_n) + 2n(n-1)S(C_n) \\
&+ \Big(Z_1(C_n) + Z_2(C_n)\Big)W(P_n) + \Big(Z_1(P_n) + Z_2(P_n)\Big)W(C_n) \\
&= \mathbf{\frac{n(n-1)}{12}(35n^3 + 22n^2 - 4n - 15)},
\end{aligned}$$

since

$W(C_n) = \frac{n^3-n}{8}$ (n odd), $\quad z_1(C_n) = 4n = z_2(C_n)$, $\quad S(C_n) = \frac{n^3-n}{2} = S^*(C_n)$,

$W(P_n) = \frac{n(n^2-1)}{6}$, $\quad z_1(P_n) = 4n - 6$, $\quad z_2(P_n) = 4n - 8$,

$S(P_n) = \frac{n(n-1)(2n-1)}{3}$, $\quad S^*(P_n) = \frac{(n-1)(2n^2-4n+3)}{3}$.

Definition

The **complete product** $G_1 \nabla G_2$ of graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, with $V_1 \cap V_2 = \emptyset$, is the graph obtained from G_1 and G_2 by joining every vertex of G_1 with every vertex of G_2.

Proposition

Let $G_i = (V_i, E_i)$ be a graph of order n_i and dimension m_i, $i = 1, 2$. The modified Schultz index of the complete product $G = G_1 \nabla G_2$ is given by

$$\begin{aligned} S^*(G) &= 4\left(m_1^2 + m_2^2\right) + 4m_1 m_2 + 3(n_1 n_2)^2 - n_1 n_2(n_1 + n_2) \\ &\quad +(6n_1 - 4 - n_2)n_2 m_1 + (6n_2 - 4 - n_1)n_1 m_2 \\ &\quad -(n_2 + 1)Z_1(G_1) - (n_1 + 1)Z_1(G_2) - Z_2(G_1) - Z_2(G_2). \end{aligned}$$

Definition

The **lexicographic product** (or **composition**) $G = G_1 \circ G_2$ of the graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ $(V_1 \cap V_2 = \emptyset)$ is the graph with vertex set $V_1 \times V_2$ and two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ being adjacent whenever $(u_1 v_1 \in E_1)$ or $(u_1 = v_1$ and $u_2 v_2 \in E_2)$.

Let $(u_1, u_2), (v_1, v_2) \in V(G)$ and $u \in V_1$.

- Degree: $d_G(u_1, u_2) = d_{G_1}(u_1) n_2 + d_{G_2}(u_2)$.
- Distances:
$$dist_G\Big((u, u_2), (u, v_2)\Big) = \begin{cases} 2 & \text{if } u_2 v_2 \in E_2 \\ 1 & \text{if } u_2 v_2 \notin E_2. \end{cases}$$
In all other cases, $dist_G\Big((u_1, u_2), (v_1, v_2)\Big) = dist_{G_1}(u_1, v_1)$.

Proposition

Let $G_i = (V_i, E_i)$ be a graph of order n_i and dimension m_i, $i = 1, 2$. The modified Schultz index of the lexicographic product $G_1 \circ G_2$ is given by

$$\begin{aligned} S^*(G_1 \circ G_2) = {} & (n_1 - 1)Z_2(G_2) + \frac{n_2^3}{2}(n_2 - 1)z_1(G_1) - \frac{1}{2}n_1 Z_1(G_2) \\ & + 4(n_2 - 1)n_2 m_1 m_2 + 2n_1 m_2^2 + \frac{n_2^3}{4}(n_2 + 3)S^*(G_1) \\ & + n_2(n_2 + 1)m_2 S(G_1) + W(G_1)(m_2^2 + \frac{1}{2}(m_2^2 + \frac{1}{2}Z_1(G_2)). \end{aligned}$$

Definition

The **subdivision graph** G' of a graph $G = (V, E)$ is obtained from G by inserting a new vertex of degree 2 in each edge of G.

Proposition

Let $G = (V, E)$ be a connected graph of order n and dimension m. The modified Schultz index of the subdivision graph G' of G is given by

$$\begin{aligned} S^*(G') &= 2S^*(G) + 4\sum_{e\in E, u\in V} d_G(u)D(u,e) \\ &+ 4m^2 + 8W(L(G)), \end{aligned}$$

where $L(G)$ is the line graph of G and for $e = xy \in E$ and $u \in V$, $D(u, e) = \min\{d_G(u, x), d_G(u, y)\}$.

Bounds on the modified Schultz index

Proposition (Andova et al., 2011)

If G is a connected graph with n vertices then

$$S^*(G) \geq 2n^2 - 5n + 3.$$

The equality holds if and only if G is the star S_n. In addition, if T is a tree (Andova et al., 2011),

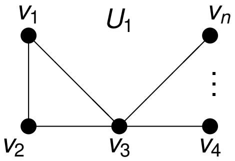
$$2n^2 - 5n + 3 = S^*(S_n) \leq S^*(T) \leq S^*(P_n) = \frac{1}{3}(2n^3 - 6n^2 + 7n - 3).$$

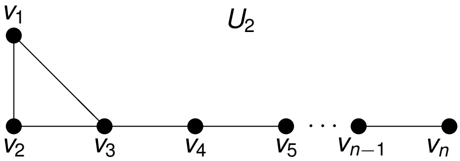
Proposition

Let $G = (V, E)$ be a unicyclic graph (that is a connected graph with $|V| = |E|$) of order n.

- For $n \geq 3$,
$$S^*(G) \geq 2n^2 + n - 9. \quad (1)$$
- (Feng and Liu, 2011) For $n \geq 5$,
$$S^*(G) \leq \frac{2}{3}n^3 - \frac{29}{3}n + 23. \quad (2)$$

The equality holds on (1) if and only if $G \simeq U_1$, and on (2) if and only if $G \simeq U_2$.





Proposition

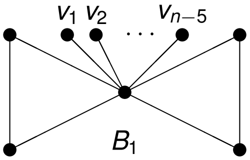
Let $G = (V, E)$ be a bicyclic graph (that is a connected graph with $|E| = |V| + 1$) of order n. For $n \geq 5$ (Chen and Liu, 2010),

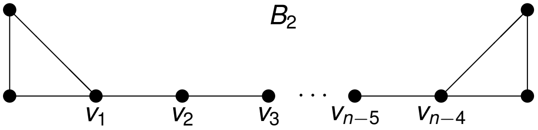
$$S^*(G) \geq 2n^2 + 7n - 13 \tag{3}$$

and for $n \geq 6$ (Feng and Liu, 2011),

$$S^*(G) \leq \frac{2}{3}n^3 + 2n^2 - \frac{53}{3}n + 27. \tag{4}$$

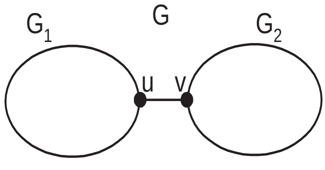
Equality holds on (3) if and only if $G \simeq B_1$, and on (4) if and only if $G \simeq B_2$.

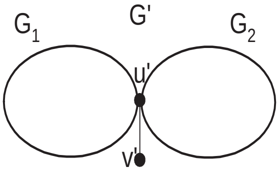




Decreasing transformations

Transformation 1:





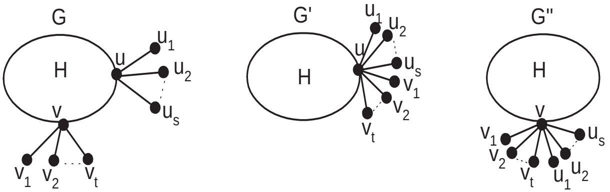
Proposition (Chen and Liu, 2010)

Let G_1 and G_2 be vertex disjoint connected graphs, $u \in V_1$, $v \in V_2$ and G is the graph obtained by connecting G_1 and G_2 with a bridge uv. Let G' be the graph obtained by coalescence of u and v in a new vertex u' and by adding a new pendant edge $u'v'$. Then

$$S^*(G') < S^*(G)$$

Decreasing transformations

Transformation 2:



Proposition (Chen and Liu, 2010)

Let H be a connected graph, $u, v \in V(H)$ and $u_1, \cdots, u_s, v_1, \cdots, v_t \notin V(H)$. Let $G = H + \{uu_1, \cdots, uu_s\} + \{vv_1, \cdots, vv_t\}$, $G' = H + \{uu_1, \cdots, uu_s\} + \{uv_1, \cdots, uv_t\}$ and $G'' = H + \{vu_1, \cdots, vu_s\} + \{vv_1, \cdots, vv_t\}$. Then

$$S^*(G) > \min\{S^*(G'), S^*(G'')\}.$$

Tricyclic graphs with 3 cycles

Tricyclic graphs

A connected graph G of order n and dimension m is a tricyclic graph if $m = n + 2$. It is known that a tricyclic graph has 3, 4, 6 or 7 cycles (see, for example, (Geng and Li, 2012)).

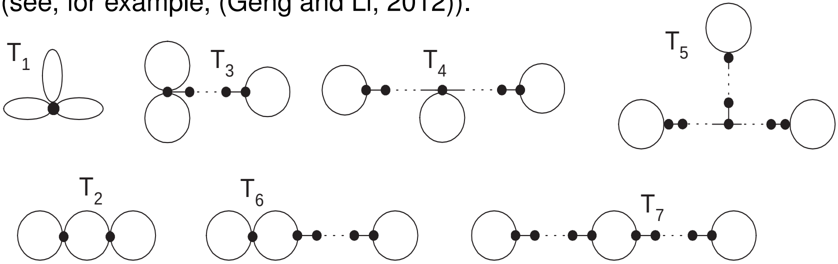
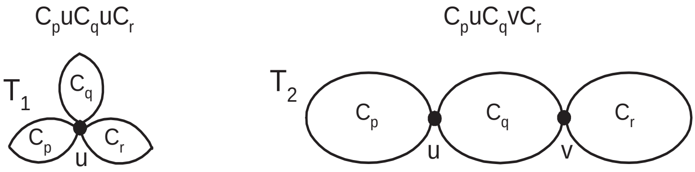


Figure: Bases of tricyclic graphs with 3 cycles

Using transformations 1 and 2 we reduce our search of a lower bound for the modified Schultz index of tricyclic graphs of order n with 3 cycles, to the study of graphs with bases T_1 and T_2, with t ($0 \leq t \leq n-7$) pendant edges attached to one vertex.

Notations:



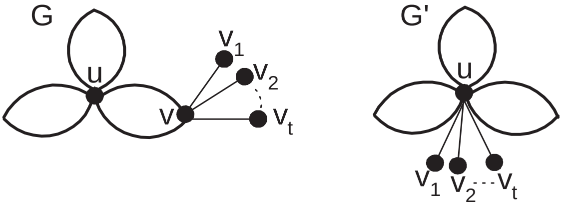
The search for the tricyclic graphs with three cycles with least modified Schultz index:

1. we determine the tricyclic graph with $n \geq 7$ vertices and three cycles of lengths p, q, r $(p + q + r \leq n - 2)$ with least modified Schultz index.
2. Using a decreasing transformation, we determine the tricyclic graphs with $n \geq$ vertices and three cycles with least modified Schultz index.

Proposition

Let $H = (V, E)$ be a $C_p u C_q u C_r$ graph. Let $v \in V \setminus \{u\}$, $G = H + \{vv_1, \cdots, vv_t\}$ and $G' = H + \{uv_1, \cdots, uv_t\}$. Then

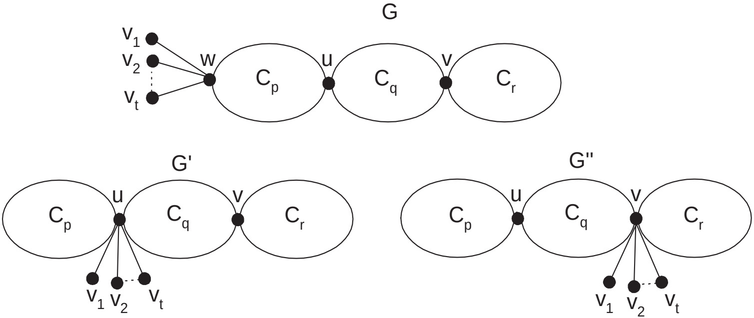
$$S^*(G') < S^*(G).$$



Proposition

Let $H = (V, E)$ be a $C_p u C_q v C_r$ graph ($u \neq v$) and $w \in V(C_p) \setminus \{u\}$. Let $G = H + \{wv_1, \cdots, wv_t\}$, $G' = H + \{uv_1, \cdots, uv_t\}$ and $G'' = H + \{vv_1, \cdots, vv_t\}$. Then

1. $S^*(G') < S^*(G)$.
2. $S^*(G'') < S^*(G')$ if and only if $p < r$.



Lemma

Let $H = (V, E)$ be a $C_p u C_q v C_r$ graph ($u \neq v$), $w \in V(C_q) \setminus \{u, v\}$, $G = H + \{wv_1, \cdots, wv_t\}$ and $G' = H + \{vv_1, \cdots, vv_t\}$. Then

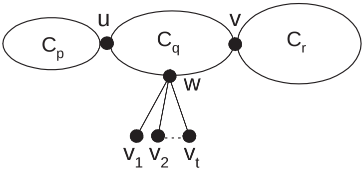
$$S^*(G') - S^*(G) = 4t\Big(- r\, dist(w, v) + p\Big(dist(u, v) - dist(u, w)\Big)\Big).$$

Corollary

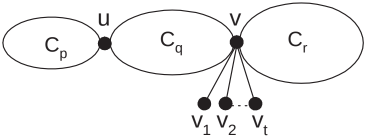
Let $H = (V, E)$ be a $C_p u C_q v C_r$ graph ($u \neq v$), $w \in V(C_q) \setminus \{u, v\}$, $G = H + \{wv_1, \cdots, wv_t\}$ and $G' = H + \{vv_1, \cdots, vv_t\}$.

1. If $p < r$ then $S^*(G') < S^*(G)$.
2. If $p = r$ then $S^*(G') \leq S^*(G)$, equality holding if and only if $dist(u, v) = dist(u, w) + dist(w, v)$.

G

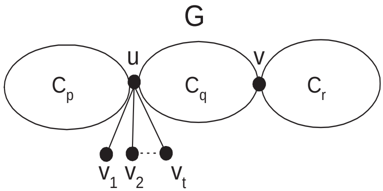


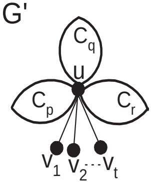
G'



Proposition

Let $H = (V, E)$ be a $C_p u C_q v C_r$ graph ($u \neq v$) and $H' = (V, E')$ be a $C_p u C_q u C_r$ graph, $G = H + \{uv_1, \cdots, uv_t\}$ and $G' = H' + \{uv_1, \cdots, uv_t\}$. Then $S^*(G') < S^*(G)$.

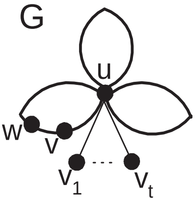


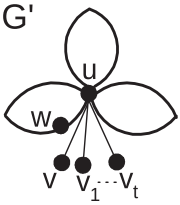


A decreasing transformation

Proposition

Let $H = (V, E)$ be a $C_p u C_q u C_r$ graph, $v \in V(C_p) \setminus \{u\}$, $N_{C_p}(v) = \{u, w\}$, $H' = (V, E')$ a $C_{p'} u C_q u C_r$ graph such that $V(C'_p) = V(C_p) \setminus \{v\}$ and $E(C'_p) = \Big(E(C_p) \setminus \{uv, vw\}\Big) \cup \{uw\}$. Let $G = H + \{uv_1, \cdots, uv_t\}$ and $G' = H' + \{uv, uv_1, \cdots, uv_t\}$. Then $S^*(G') < S^*(G)$.





Theorem

If G is tricyclic graph with 3 cycles and $n \geq 7$ vertices then

$$S^*(G) \geq 2n^2 + 9n - 5$$

with equality if and only if $G \simeq S_n(3,3,3)$.

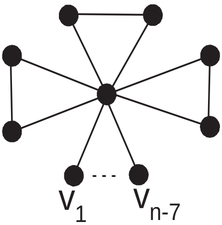


Figure: Tricyclic graph $S_n(3,3,3)$

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