Merrifield-Simmons index of Graphs

E-seminar, IIT- Kharagpur

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Introduction.

Notations

- G Simple Connected graph.
- m Number of edges of graph G.
- n Number of vertices of graph G.
- $d(v_i)$ Degree of vertex v_i.
- d_{v_i} Degree of vertex v_i.
- Δ Maximum degree of graph.
- δ Minimum degree of graph.

Mathematical chemistry

1. Chemical graph theory
    1. Topological indices

Topological index is a numerical value which associate with a graph structure

1. Degree Based Indices

1. Degree Based Indices
2. Distance Based Indices

1. Degree Based Indices
2. Distance Based Indices
3. Energy Based Indices

1. Degree Based Indices
2. Distance Based Indices
3. Energy Based Indices

1. Graph Invarients based counting subsets

Independent edge subsets

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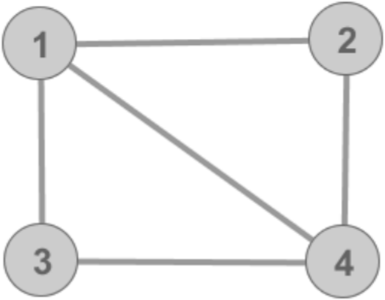
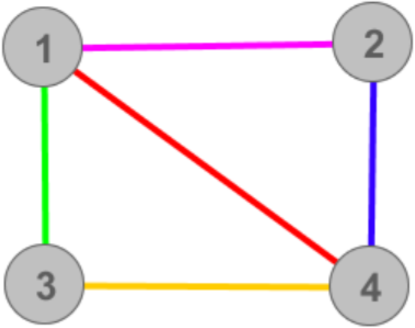
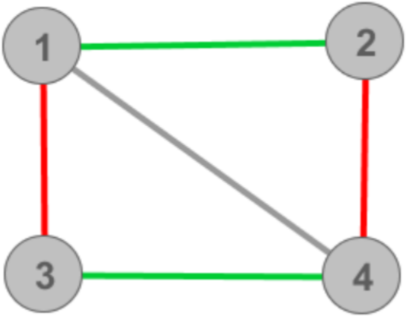
Let $m(G, k)$ denotes the number of $k-$matchings in $G, k \geq 1$



The simple connected Graph G_1



single-edge sets: 5



Two-Matchings : 2
(1 red pair and 1 green pair of edges.)

Independent edge subsets

$$z(G) = \sum_{k \geq 0} m(G, k),$$

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$$z(G_1) = 1 + 5 + 2 = 8.$$

The quantity $z(G)$ associated with a graph was introduced to the chemical literature in 1971 by the Japanese chemist **Haruo Hosoya**.

Haruo Hosoya

Hosaya Index $z(G)$

Given a graph G, a $k-$independent set is a set of k vertices, no two of which are adjacent.

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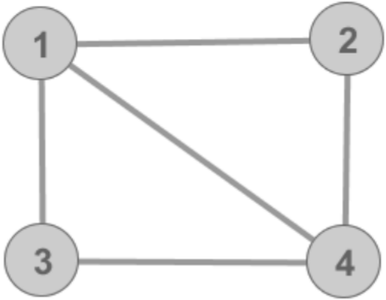
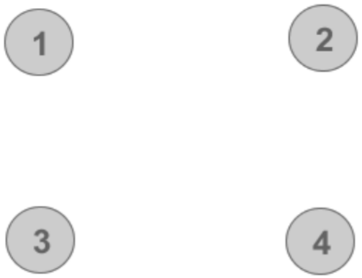
The empty set is an independent set.

It is both consistent and convenient to define $i(G,0) = 1$.



The simple connected Graph G_1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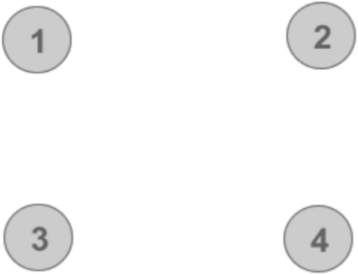
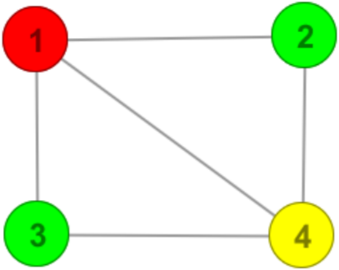


Single vertex set: 4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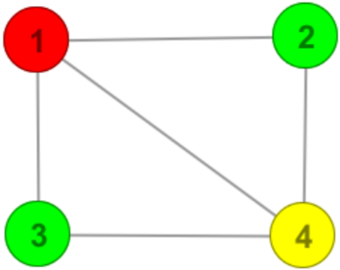
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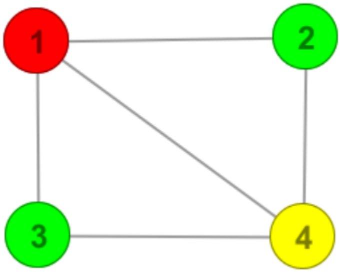

Independent set of two vertices: 1

The total number of independent vertex sets (including the empty vertex set) of a graph $G = (V, E)$ denoted by $i(G)$.

$$i(G) = i(G, 0) + i(G, 1) + \ldots + i(G, k)$$

$$i(G) = \sum_{k \geq 0} i(G, k)$$

$$i(G_1) = 1 + 4 + 1 = 6.$$

The quantity $i(G)$ associated with a graph was introduced to the chemical literature in 1980 by the chemists Richard E. Merrifield and Howard E. Simmons .

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Merrifield-Simmons index $i(G)$.

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The number of independent sets occurred in this framework as the number of open sets of a certain finite topology, and of all the aspects of their theory, it probably received the most attention.

In chemical literature, the total number of the independent sets of graphs $i(G)$ is referred to as the Merrifield-Simmons index.

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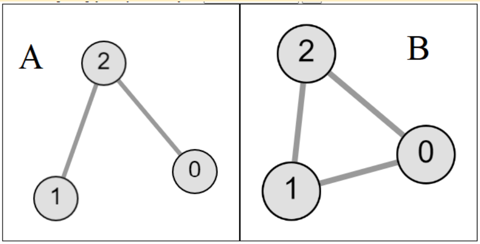
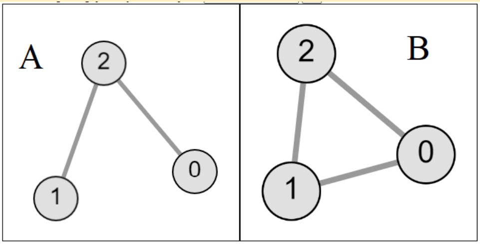
In chemical literature, the total number of the matchings of graphs $z(G)$ is referred to as the Hosaya index.

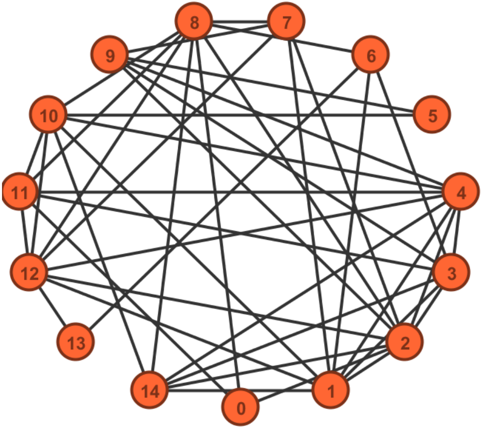
3 vertices



3 vertices

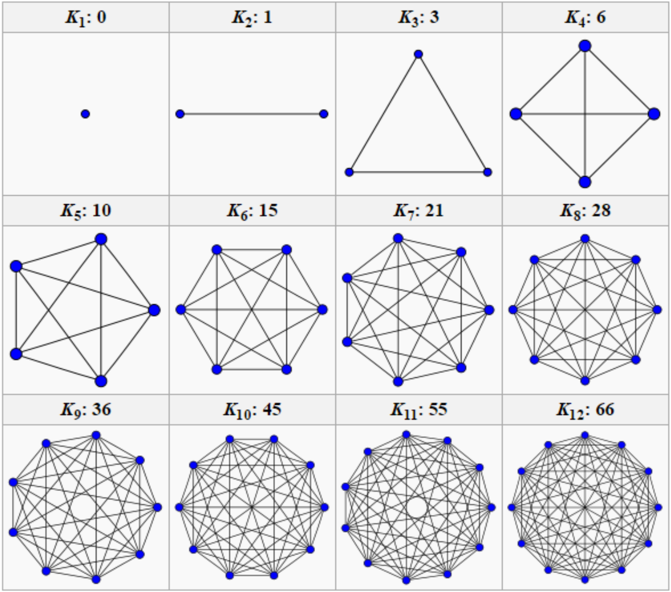


$$i(A) = 1 + 3 + 1 = 5 \qquad i(B) = 1 + 3 = 4$$

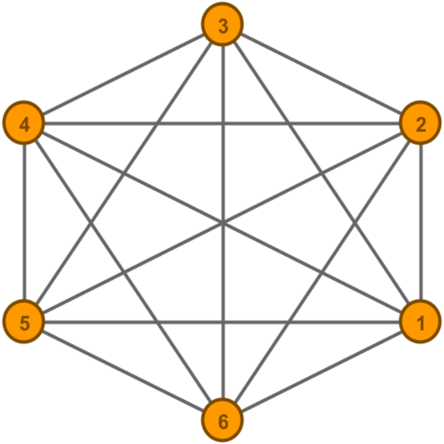


Simple connected graph G_1 on 15 vertices.

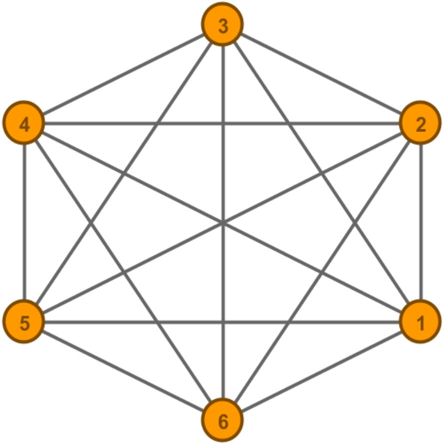
Complete Graphs K_n.



Complete Graph K_6.

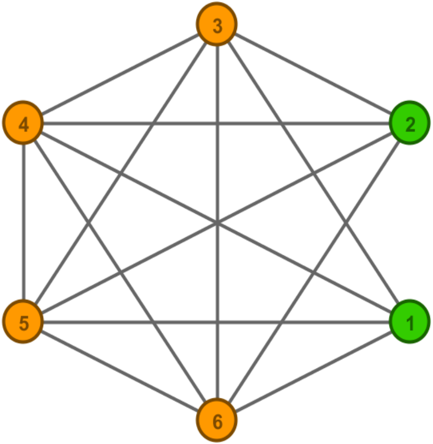


Complete Graph K_6.

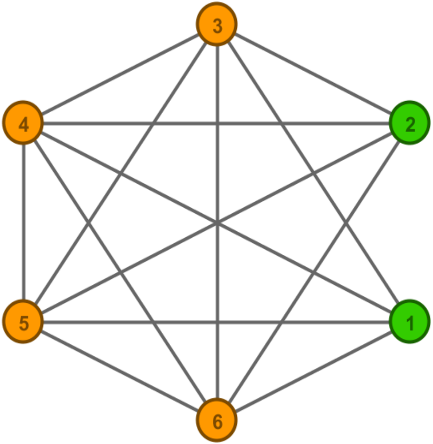


$$i(K_6) = 7$$

Complete Graph $K_6 - e$.

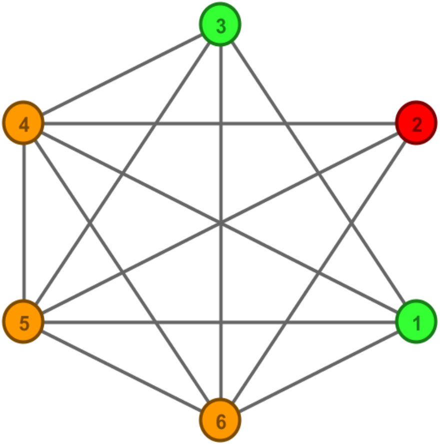


Complete Graph $K_6 - e$.

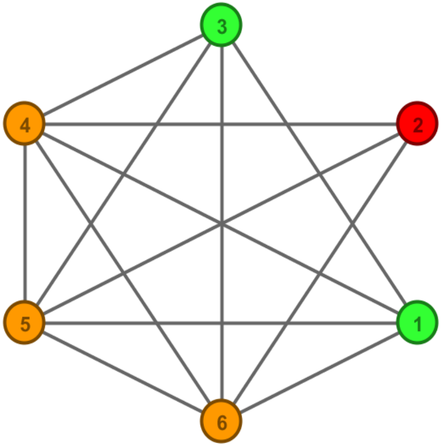


$$i(K_6 - e) = 8$$

Complete Graph6 $K_6 - 2e$.

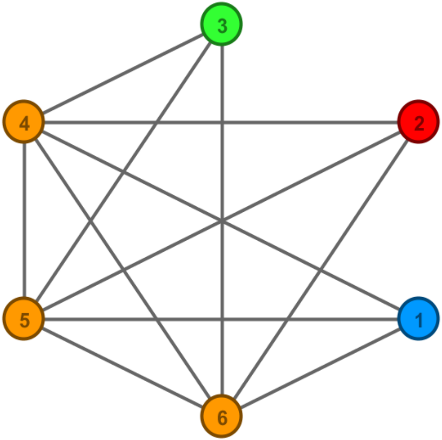


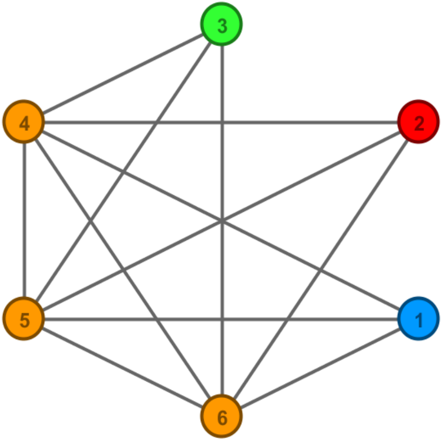
Complete Graph6 $K_6 - 2e$.



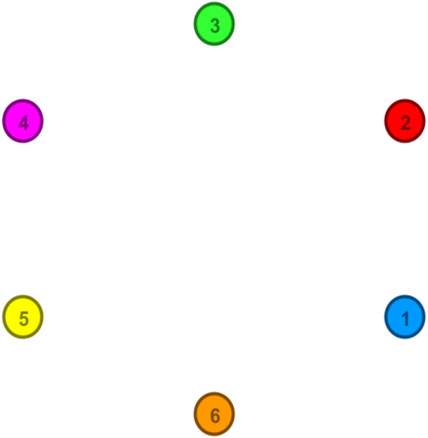
$$i(K_6 - 2e) = 9$$

Complete Graph $K_6 - 3e$.





$$i(K_6 - 2e) = 11$$


3
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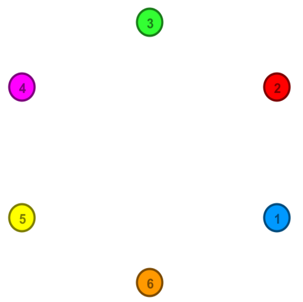

$$
\begin{aligned}
i(E_6) &= 1 + 6C_1 + 6C_2 + 6C_3 + 6C_4 + 6C_5 + 6C_6 \\
&= 1 + 6 + 15 + 20 + 15 + 6 + 1 \\
&= 64
\end{aligned}
$$

Observation: If edges are removed from a graph, then the Merrifield- Simmons index $i(G)$ increases.

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Lemma 1

Let G_1 and G_2 be two graphs. If G_1 can be obtained from G_2 by deleting some edges, then $i(G_2) < i(G_1)$.

For any simple graph G.

Theorem 2

For every graph G with n vertices, we have

$$n + 1 = i(K_n) \leq i(G) \leq i(E_n) = 2^n,$$

equality in the first inequality only holds if G is complete, and equality in the second inequality only holds if G is edgeless.

If G is a simple connected graph.

If G is a simple connected graph, then

$$?? \leq i(G) \leq ??$$

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If G is a simple connected graph, then

$$K_n \leq i(G) \leq ??$$

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$$K_n \leq i(G) \leq ??$$

Complete graph on n vertices.

$$i(K_n) = n + 1$$

Let G be a simple connected graph on n vertices and m edges. Then

$$n - 1 \leq m \leq \frac{n(n-1)}{2}$$

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Complete graph K_n $\rightarrow$ Tree T_n

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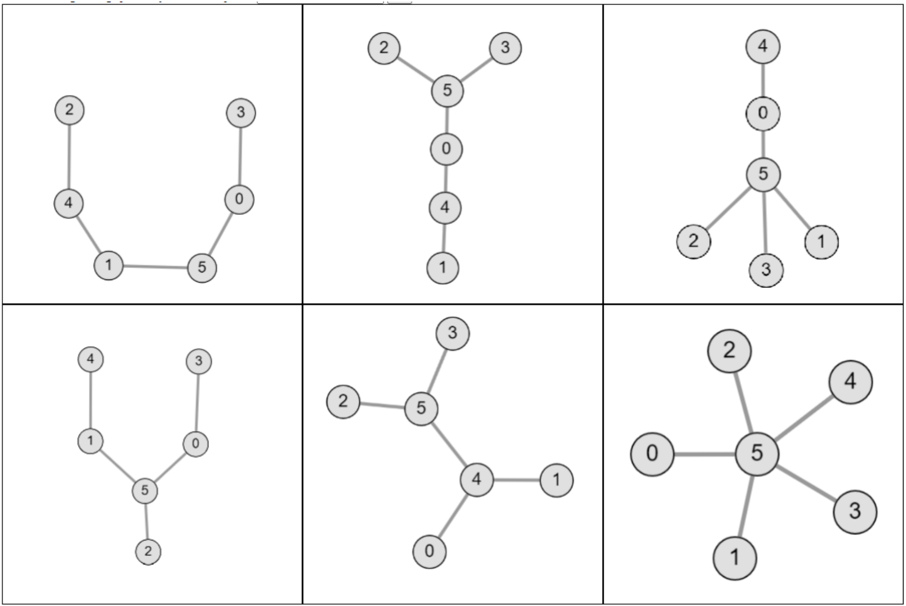
Complete graph $K_n \rightarrow$ Tree T_n

$$n + 1 = i(K_n) \leq i(G) \leq i(T_n)$$

Trees on 6 Vertices



H. Prodinger and R. F. Tichy, Fibonacci numbers of graphs, The Fibonacci Quarterly, 20(1) (1982) 16-21.

Fibonacci Number	Values
F_0	1
F_1	1
F_2	2
F_3	3
F_4	5
F_5	8
F_6	13
F_7	21
F_8	34
F_9	55
F_{10}	89

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F_8	34
F_9	55
F_{10}	89

$$F_n = F_{n-1} + F_{n-2}$$

Construct the total number of subsets of $\{1, \ldots, n\}$ such that no two elements are adjacent are:

$$\{1\} := \{\phi, \{1\}\} \; Count : 2$$

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$$\{1,2,3\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\}, \{3\} \\ \{1,3\} \end{array} \right\} \mathit{Count} : 5$$

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$$\{1,2\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\} \end{array} \right\} Count : 3$$

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$$\{1,2,3,4\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\}, \{3\}, \{4\} \\ \{1,3\}, \{2,4\}, \{1,4\} \end{array} \right\} Count : 8$$

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$$\{1,2\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\} \end{array} \right\} \mathit{Count} : 3$$

$$\{1,2,3\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\}, \{3\} \\ \{1,3\} \end{array} \right\} \mathit{Count} : 5$$

$$\{1,2,3,4\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\}, \{3\}, \{4\} \\ \{1,3\}, \{2,4\}, \{1,4\} \end{array} \right\} \mathit{Count} : 8$$

$$\{1,2,3,4,5\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \\ \{1,3\}, \{1,4\}, \{1,5\}, \{2,4\}, \{2,5\}, \{3,5\} \\ \{1,3,5\} \end{array} \right\} \mathit{Count} : 13$$

Construct the total number of subsets of $\{1, \ldots, n\}$ such that no two elements are adjacent are:

$$\{1\} := \{\phi, \{1\}\} \; Count : 2$$

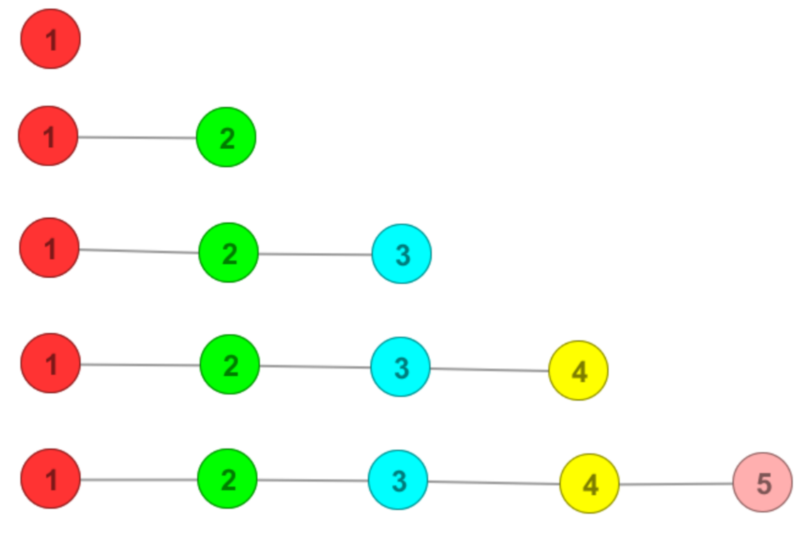
$$\{1,2\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\} \end{array} \right\} Count : 3$$

$$\{1,2,3\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\}, \{3\} \\ \{1,3\} \end{array} \right\} Count : 5$$

$$\{1,2,3,4\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\}, \{3\}, \{4\} \\ \{1,3\}, \{2,4\}, \{1,4\} \end{array} \right\} Count : 8$$

$$\{1,2,3,4,5\} := \left\{ \begin{array}{l} \phi \\ \{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \\ \{1,3\}, \{1,4\}, \{1,5\}, \{2,4\}, \{2,5\}, \{3,5\} \\ \{1,3,5\} \end{array} \right\} Count : 13$$

Path



Chemical graph

$i(G)$	Values
$i(P_1)$	2
$i(P_2)$	3
$i(P_3)$	5
$i(P_4)$	8
$i(P_5)$	13

F_n	Values	$i(G)$	Values
F_0	1		
F_1	1		
F_2	2	$i(P_1)$	2
F_3	3	$i(P_2)$	3
F_4	5	$i(P_3)$	5
F_5	8	$i(P_4)$	8
F_6	13	$i(P_5)$	13
F_7	21	$i(P_6)$	21
F_8	34	$i(P_7)$	34

F_n	Values	$i(G)$	Values
F_0	1		
F_1	1		
F_2	2	$i(P_1)$	2
F_3	3	$i(P_2)$	3
F_4	5	$i(P_3)$	5
F_5	8	$i(P_4)$	8
F_6	13	$i(P_5)$	13
F_7	21	$i(P_6)$	21
F_8	34	$i(P_7)$	34

$$i(P_n) = F_{n+1}$$

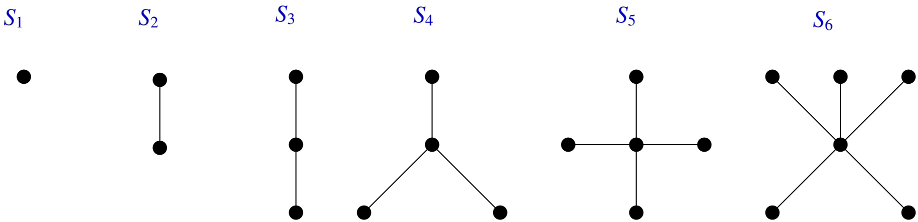
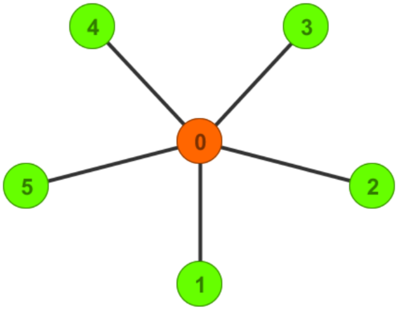


Figure : Examples for the star S_n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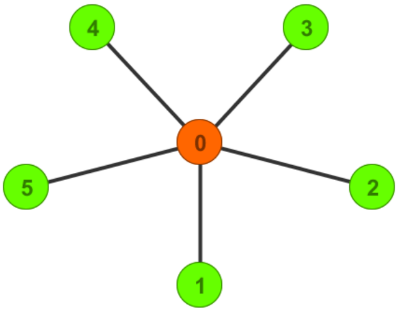


$$i(S_n) = 1 + n + (n-1)C_2 + (n-1)C_3 + \ldots + (n-1)C_{n-1}$$

$$i(S_n) = 1 + 1 + (n-1)C_1 + (n-1)C_2 + (n-1)C_3 + \ldots + (n-1)C_{n-1}$$

$$i(S_n) = 1 + 2^{n-1}$$

We Know that. $nC_0 + nC_1 + nC_2 + \ldots + nC_n = 2^n$

The Fibonacci number $F(S_n)$ can be computed by counting the number of admissible vertex subsets (they do not contain two adjacent vertices) containing the vertex n or not containing n. Thus

$$F(S_n) = 1 + 2^{n-1}.$$

$$i(S_n) = 1 + 2^{n-1}.$$

Theorem 3

For every tree T with n vertices, we have

$$F_{n+1} = i(P_n) \leq i(T) \leq i(S_n) = 2^{n-1} + 1,$$

with right equality holds if and only if T is a star S_n and the left equality holds if and only if T is a path P_n.

If G is a simple connected graph.

If G is a simple connected graph, then

$$?? \leq i(G) \leq ??$$

If G is a simple connected graph.

If G is a simple connected graph, then

$$?? \leq i(G) \leq ??$$

$$n + 1 = i(K_n) \leq i(G) \leq i(S_n) = 1 + 2^{n-1}.$$

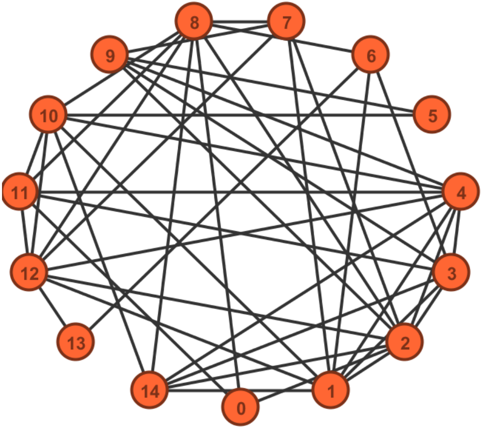
If G is a simple connected graph.

Theorem 4

Let G be a simple connected graph, then

$$n+1 = i(K_n) \leq i(G) \leq i(S_n) = 1 + 2^{n-1}.$$

Equality in the first inequality holds if and only if $G \cong K_n$ and the equalilty in the second inequality holds if and only if S_n.



Simple connected graph G_1 on 15 vertices.

$$i(G_1) = ???.$$

I. Gutman, O.E. Polansky, Mathematical Concept in Organic Chemistry, Springer, Berlin, 1986.

Lemma 5

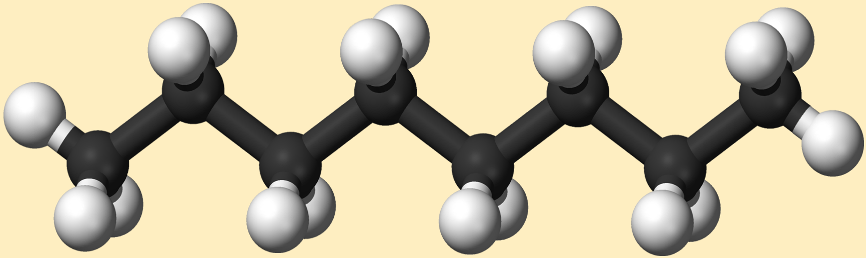
Let $G = (V, E)$ be a graph.

(i) *If* $uv \in E(G)$, *then* $i(G) = i(G - uv) - i\Big(G - \{N[u] \cup N[v]\}\Big)$.

(ii) *If* $v \in V(G)$, *then* $i(G) = i(G - v) + i(G - N[v])$.

(iii) *If* $G_1, G_2, \ldots, G_t$ *are the connected components of the graph G, then*

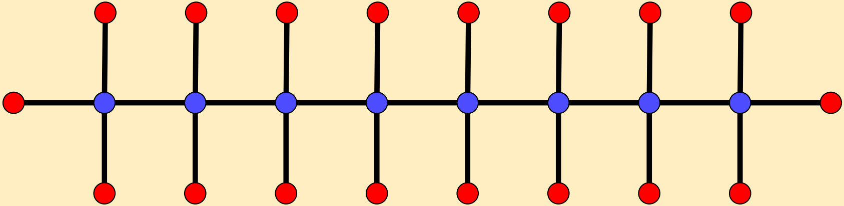
$$i(G) = \prod_{j=1}^{t} i(G_j).$$



In chemical graph theory, the molecular structure of a compound is often presented with a graph, where the atoms are represented by vertices and bonds are represented by edges.

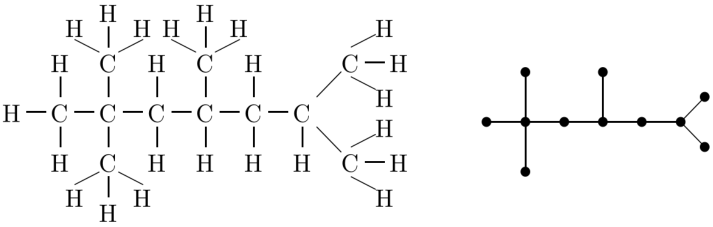
Graph representation for the above chemical structure

Blue refers Carbon atoms, Red refers Hydrogen atoms.



Molecular Graph

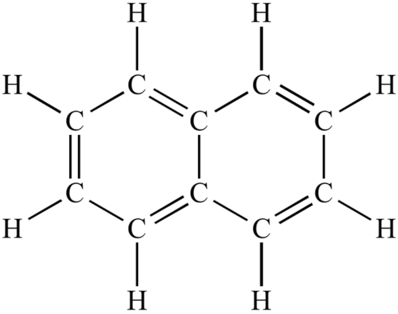
Molecular Graph



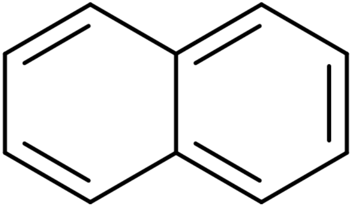
Structural formula for 2,2,4,6-tetramethylheptane (on the left) and its corresponding molecular graph (on the right).

Naphthalene Balls

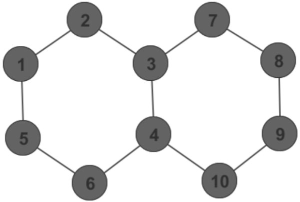
Naphthalene Structure



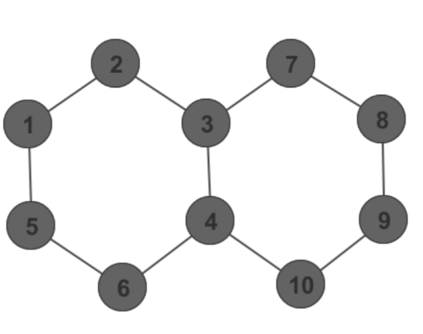
Naphthalene Structure



Chemical graph



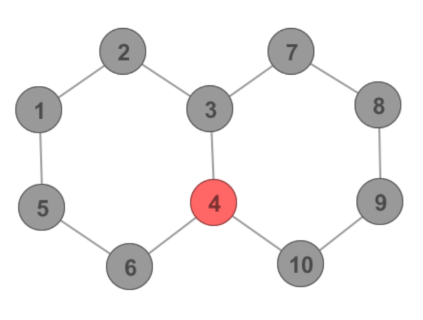
Chemical graph



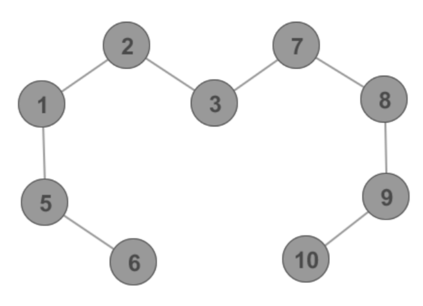
Naphthalene N.

Calculate $i(N)$

Chemical graph



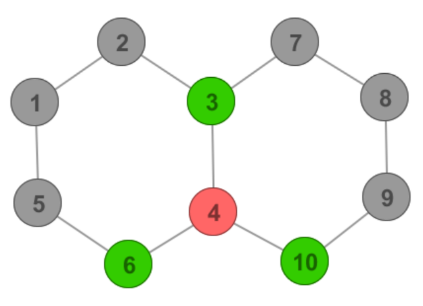
Chemical graph



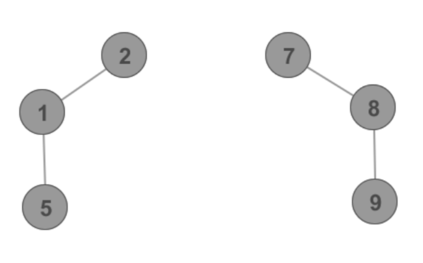
$$N - \{4\}$$

$$i(N - \{4\}) = i(P_9) = F_{10} = 89$$

Chemical graph



Chemical graph



$$N - \{3, 4, 6, 10\}$$

$$i(N - \{3, 4, 6, 10\}) = i(P_3) * i(P_3) = F_4 * F_4 = 5 * 5 = 25$$

$$i(N) = i(N - \{4\}) + i(N - \{\text{Neighbors of } 4\})$$

$$i(N) = i(N - \{4\}) + i(N - \{3, 4, 6, 10\}) = 89 + 25 = 114$$

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$$i(N) = 114$$

H.Hua, X. Xu, H. Wang, Unicyclic Graphs with Given Number of Cut Vertices and the Maximal Merrifield - Simmons Index, Filomat 28:3 (2014) 451-461.

Theorem 6

Let T be a tree, not isomorphic to S_n, with n vertices. Then

$$i(T) \leq 3(2^{n-3}) + 2,$$

with equality if and only if $T \cong D_{1,n-3}$.

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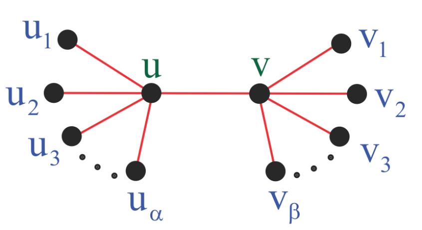

Double Star $D_{\alpha,\beta}$.

Y. Hu, Y. Wei, The number of independent sets in a connected graph and its complement, The Art of Discrete and Applied Mathematics 1 (2018) 1-10.

Theorem 7

Let T be a tree of order n with connected complement $\overline{T}$, then

$$i(T) + i(\overline{T}) \geq 2n + F_{n+1}$$

with equality if and only if $T \cong P_n$, where F_{n+1} is the Fibonacci Number.

Theorem 8

Let T be a tree of order n with connected complement $\overline{T}$, then

$$i(T) + i(\overline{T}) \leq 2 + 2n + 2n^{n-3} + 2^{n-2}$$

with equality if and only if $T \cong D_{1,n-3}$.

Theorem 9

If G is a unicyclic graph of order n, then

$$i(G) \geq F_{n-1} + F_{n+1}$$

and equality occurs if and only if $G \cong C_n$ or $G \cong L_{n,3}$.

Theorem 9

If G is a unicyclic graph of order n, then

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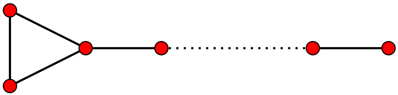

$L_{n,3}$

Theorem 10

If G is a unicyclic graph of order n, then

$$i(G) \leq 3 * 2^{n-3} + 1$$

and equality holds if and only if G is a C_4 or $G \cong S_n^+$.

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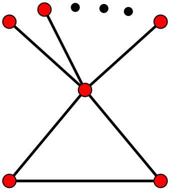

Theorem 11

If G is a bicyclic graph of order n, then

$$i(G) \leq 5 * 2^{n-4} + 1$$

, equality holds if and only if $G \cong B_1$.

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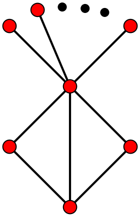
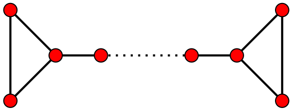


Theorem 12

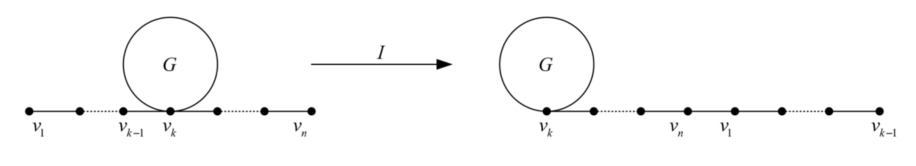
If G is a bicyclic graph of order n, then

$$i(G) \geq 5 * F_{n-2}$$

, equality holds if and only if $G \cong B_2$.

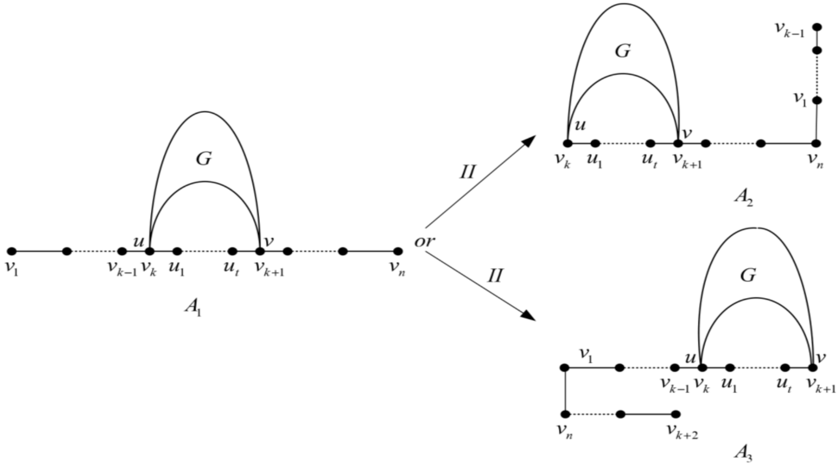


Transformation I



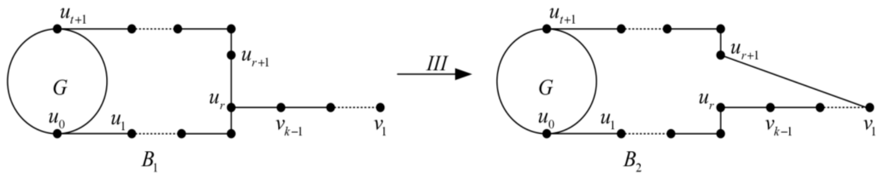
Let G_1 and G_2 be the graphs in Transformation I. Then $i(G_1) > i(G_2)$.

Transformation II



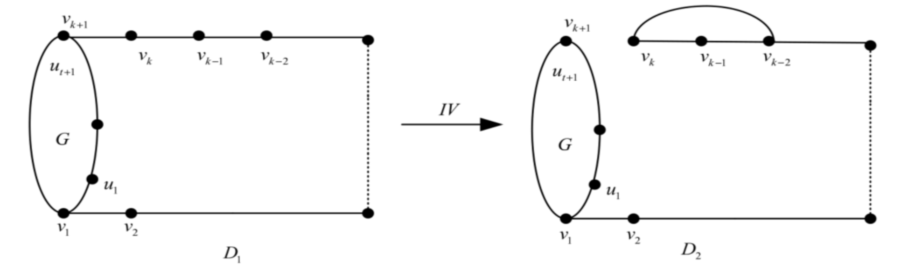
Let A_1, A_2 and A_3 be the graphs in Transformation II. Then $i(A_1) > i(A_2)$ or $i(A_1) > i(A_3)$.

Transformation III



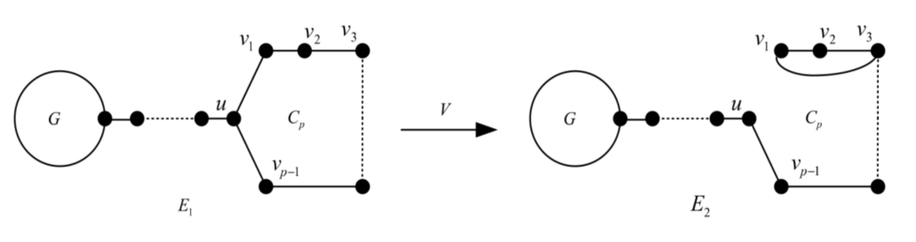
Let B_1 and B_2 be the graphs in Transformation III. Then $i(B_1) > i(B_2)$

Transformation IV



Let D_1 and D_2 be the graphs in Transformation IV. Then $i(D_1) > i(D_2)$.

Transformation V



Let E_1 and E_2 be the graphs in Transformation V. Then $i(E_1) > i(E_2)$.

Results connecting $i(G)$ with other distance based topological indices.

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H. Hua, X. Hua, H. Wang, Further results on the Merrifield-Simmons index, Discrete Applied Mathematics, 283 (2020) 231-241.

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Let G be a simple connected graph of order n with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ and edge set $E(G)$. Let $d_1 \geq d_2 \geq d_3 \geq ... \geq d_n$ be the degree sequence of G.

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Graph Matrices: Adjacency matrix:

$$A(G) := [a_{ij}]_{n\times n}, a_{ij} = \begin{cases} 1 & \text{if } \mathrm{v_i v_j} \in \mathrm{E(G)} \\ 0 & \textit{otherwise} \end{cases}$$

Degree diagonal matrix: $D(G) := diag(d_1, d_2, ..., d_n)$.

Laplacian Matrix: $L(G) := D(G) - A(G)$.

Signless Laplacian Matrix: $Q(G) := D(G) + A(G)$.

Adjacency spectrum: $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$.

Laplacian spectrum : $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n = 0$.

Signless Laplacian spectrum : $q_1 \geq q_2 \geq \ldots \geq q_n$.

Milan Randić

Randić Index

In 1975, M. Randić introduces the connectivity index, defined by

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

P. Hansen, C. Lucas, Bounds and conjectures for the signless Laplacian index of graphs, Linear Algebra Appl. 432 (2010) 3319-3336.

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Conjectures

Let G be a connected graph on $n \geq 4$ vertices with signless Laplacian index q_1 and Randić index R. Then

Conjecture 1

$$q_1 - R \leq \frac{3}{2}(n-2)$$

equality holds if and only if $G \cong K_n$.

Conjecture 2

$$\frac{q_1}{R} \leq \begin{cases} \dfrac{4n-4}{n}, & 4 \leq n \leq 12, \\ \dfrac{n}{\sqrt{n-1}}, & n \geq 13, \end{cases}$$

equality holds if and only if $G \cong K_n$, for $4 \leq n \leq 12$ and for S_n for $n \geq 13$.

Proofs supporting Conjecture 1

H. Deng, S. Balachandran, S. Ayyaswamy, On two conjectures of Randić index and the largest signless Laplacian eigenvalue of graphs, J. Math. Anal. Appl. 411 (1) (2014) 196-200.

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Proofs supporting Conjecture 2

B. Ning, X. Peng The Randić index and signless Laplacian spectral radius of graphs, Discrete Mathematics 342 (2019) 643 - 653.

Boris Furtula

Geometric-Arithmetic Index

In 2009, Vukičević and Furtula introduced a new class of topological index, named the geometric-arithmetic index, defined by

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}.$$

M. Aouchiche, P. Hansen, Comparing the GeometricArithmetic Index and the Spectral Radius of Graphs, MATCH Commun. Math. Comput. Chem. 84 (2020) 473-482.

Conjecture

For any connected graph G on $n \geq 8$ vertices with spectral radius λ_1 and geometric-arithmetic index GA, Randić index R,

$$\frac{GA}{\lambda_1^2} \leq \frac{R}{2},$$

with equality if and only if G is the cycle C_n.

Z. Du, B. Zhou, On Quotient of Geometric-Arithmetic Index and Square of Spectral Radius, MATCH Commun. Math. Comput. Chem. 85 (2021) 77-86.

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Theorem 13

Let $r \geq 2$ be a fixed integer, and x_r the largest positive root of the equation

$$(x - 3 + 2\sqrt{2}) \cos^r \frac{\pi}{x+1} = x - 3 + \frac{4\sqrt{2}}{3}$$

For any connected graph G on $n > x_r$ vertices, we have

$$\frac{GA}{\lambda_1^r} \leq \frac{R}{2^{r-1}},$$

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Set $r = 2$. Note that $x_2 \approx 7.66251$. It is then reduced to the solution of the conjecture.

Relation between $i(G)$ with λ_1, μ_1, or q_1 is still unexplored.


Thank You!