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Original Research Article

Randic and General Randic Indcies of Unicyclic Graphs

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Abstract : Let a simple graph G is a connected graph. The General Randic Index GR(G) of a graph G is defined as

$$GR(G) = \sum (\rho_u \rho_v)^t ; \qquad uv \in E(G)$$

where ρ_u and ρ_v are the degree of vertices u and v. If $t = \frac{-1}{2}$,then it is called Randic index which is defined as:-

$$uv \in E(G) \qquad R(G) = \sum \frac{1}{\sqrt{\rho_u \rho_v}}$$

In this paper, we construct the Randic and General Randic Indcies of Alkanes and unicyclic graphs with application to cycloalkanes.

Keywords: Randic , General Randic Indcies, Alkanes, Unicyclic Graphs and Cycloalkanes

INTRODUCTION

A graph G(V,E) is a nonempty finite set V(G) with another set E(G) (possibly empty) which consists pairs of elements in V(G). In chemical graphs, the vertices correspond to the atoms of the molecule, and the edges correspond to the bonds .

A topological representation of a molecule can be carried out through a molecular graph. The descriptors is a real number descriptor of the molecular constructing obtained from the chance of (hydrogen – depleted) molecular graph.

Let G be a simple graph, then we have two important types of topological indices

The first type is called degree_ based topological indices, for example, Atom-bond connectivity Index, Harmonic Index and Sum-connectivity Index et.al.

The second type is called distance – based topological indices for example The Szeged Index and The Wiener Index et.al.

There are many different kinds of topological indices[1-8]. One of them is the Randic Index.

In 1975, the chemist Milan Randic[5] proposed this index for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons.

The Randic Index R(G) of a nontrivial connected graph G(V,E) is defined as :

$$R(G) = \sum_{UV\in E(G)} \frac{1}{\sqrt{\rho_u \rho_v}}.$$

Here ρ_u and ρ_v are the degrees of vertices u and v, respectively.

Motivated by the Randic index , in 1998 B. Bollobas and p.Erdos [1] introduced the General Randic Index:

$$GR(G) = \sum(\rho_u \rho_v)^t$$

Where (t) is any real number.

In 2003, Huiqing liu,..et al, Studied the mistake in the proof of their result [Let G=(v,E)be a trianle-free graph of order n with (G)≥ 2 Then R(G)≥ $\sqrt{2(n-2)}$.

In 2003, Xueliang Li and Yongtang Shi, Studied the upper and lower bounds for the general Randic index among graphs with n vertices and the corresponding extremal graph.

In 2007, Xueliang Li and Yongtang Shi Studied the results Known for the (general)Randic index of chemical graph.

RANDIC AND GENERAL RANDIC INDICES OF ALKANES GRAPH

In this section, we provide the Randic and General Randic Indices of alkanes. Alkanes are hydrocarbons with only a single bonds between the atoms, and it has Formula C_nH_{2n+2}, where n is number of carbon atoms. (see Fig. 1)

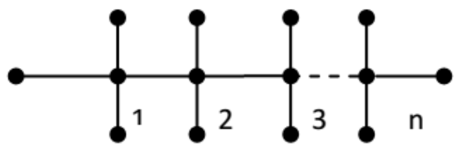

Fig. 1. Alkanes

Theorem 2.1. Let n be a positive integer number where n ≥ 1, the General Randic Index and the Randic index of a graph G = $C_n H_{2n+2}$ are:

$$GR(G) = (n-1)(16)^t + (2n+2)(4)^t$$
$$R(G) = \frac{n-1}{4} + \frac{2n+2}{2}$$

Proof:- we have 3n+1 edges. (n−1) edges are incidents on a vertex u with $\rho(u) = 4$ and a vertex v with $\rho(v) = 4$. (2n+2) edges are incidents on a vertex u with $\rho(u) = 1$ and a vertex v with $\rho(v) = 4$.

Hence by definition of General Randic Index we get the following:

$$GR(G) = (n-1)(16)^t + (2n+2)(4)^t$$

If $t = -\frac{1}{2}$ then it is called Randic index

$$R(G) = \frac{n-1}{4} + \frac{2n+2}{2}$$

Remark: If G is isomerism of alkanes, the General Randic Index and the Randic index of G is the same as Alkanes above. That are:

$$GR(G) = (2n+2)(4)^t + (n-1)(16)^t$$
$$R(G) = \frac{2n+2}{2} + \frac{n-1}{4}$$

RANDIC AND GENERAL RANDIC INDICES OF UNICYCLIC GRAPHS

In this section, we study the Randic and General Randic Indices of Unicyclic graphs.

Let U_n^p be a unicyclic graph if it is connected and has the same number of vertices and edges (see Fig. 2.)

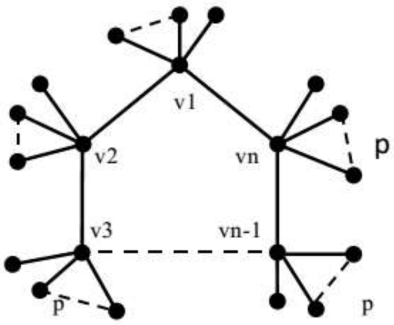

Fig. 2. A unicyclic graph U_n^p

Theorem 3.1. Let n and p be positive integer numbers with n ≥ 3, p ≥ 1, the General Randic index and the Randic index of Uincyclic graph U_n^p are:

$$\mathbf{GR}(U_n^p) = n(P+2)^{2t} + np(p+2)^t$$
$$\mathbf{R}(U_n^p) = \frac{n}{p+2} + \frac{np}{\sqrt{p+2}}$$

Proof:- we have (n+ np) edges. n edges of them are incidents on a vertex $u \; with \; \rho(u) = (p+2) \; and \; a \; vertex \; v \; \rho(v) = (p+2)$. np edges of them are incidents on a vertex $u \; with \; \rho(u) = 1 \; and \; a \; vertex \; v \; \rho(v) = (p+2)$.

Hence by definition of General Randic Index, we get the following:

$$GR\left(U_n^p\right) = n(P+2)^{2t} + np(p+2)^t$$

If $t = -\frac{1}{2}$ then it is called Randic index

$$R(G) = \frac{n}{p+2} + \frac{np}{\sqrt{p+2}}$$

In Theorem 3.2. if p=2 we get the following Cycloalkanes, denoted by U_n^{*2} with chemical formula (C_nH_{2n}). (see Fig. 3.)

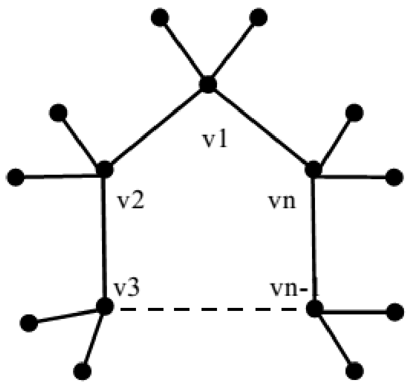

Fig.3. Cycloalkanes U_n^{*2}

Corollary:- Let n be a positive integer number the General Randic index and Randic index of Cycloalkanes U_n^{*2} are:-

$$\mathbf{GR}(U_n^{*2}) = \boldsymbol{n}(\mathbf{4})^{2t} + \mathbf{2}\boldsymbol{n}(\mathbf{4})^{t}$$
$$\boldsymbol{R}(U_n^{*2}) = \frac{\boldsymbol{n}}{\mathbf{4}} + \frac{\mathbf{2}\boldsymbol{n}}{\mathbf{2}}$$

Proof : The proof is clearly of proof theorem 3.2 by letting p=2.

Alkyl or branches of alkyl are a chemical compound with the chemical formula (C_nH_{2n+1}). They are classes of alkanes. If n ≥ 1 we get the followingthe followingon branches of alkyl. For example:
If n = 1, it is called Methyl (CH_3)
If n = 2, it is called ethyl (C_2H_5)
If n = 3 ,it is called propyl (C_3H_7)
(see Fig.4.)

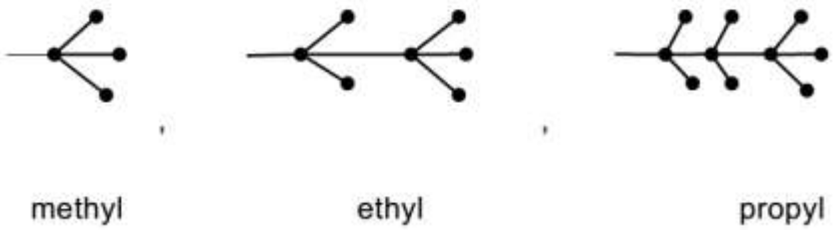

Fig.4. Some types of branches of alkyl

Theorem 3.3. Let n be a positive integer number. The General Randic Index and the Randic index of alkyl or branches of alkyl (C_nH_{2n+1}) are:

$$\boldsymbol{GR}(\boldsymbol{G}) = \begin{cases} \mathbf{3}(\mathbf{3})^{t} & \boldsymbol{if\ n} = \mathbf{1} \\ \mathbf{2}(\mathbf{3})^{t} + (\mathbf{12})^{t} + (\boldsymbol{n}-\mathbf{2})(\mathbf{16})^{t} + (\mathbf{2}\boldsymbol{n}-\mathbf{1})(\mathbf{4})^{t} \end{cases}$$

$$\mathrm{R(G)}= \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{12}} + \frac{2n-1}{2} + \frac{n-2}{4}$$

Proof:- we have two cases

Case 1. If n = 1, then we have three edges every edge is an incident on a vertex u with $\rho(u) = 1$ and a vertex v with $\rho(v) = 3$

Hence by definition of General Randic index; we get the following:

$$GR(G) = 3(3)^t$$

$If\ t = -\frac{1}{2}\ then\ it\ is\ called\ Randic\ Index$

$$R(G) = \frac{\mathbf{3}}{\sqrt{\mathbf{3}}}$$

Case 2. We have 3n edges. Two edges of them are incidents on a vertex u with $\rho(u) = 3$ and a vertex v with $\rho(v) = 1$, one edge of them is an incident on a vertex u with $\rho(u) = 3$ and a vertex v with $\rho(v) = 4$, (2n – 1) edges of them are incidents on a vertex u with $\rho(u) = 4$ and a vertex v with $\rho(v) = 1$, (n – 2) edges of them are incidents on a vertex u with $\rho(u) = 4$ and a vertex v with $\rho(v) = 4$.

Hence by definition of General Randic Index, we get the following:

$$\mathbf{GR(G)} = 2(3)^t + (12)^t + (n-2)(16)^t + (2n-1)(4)^t$$

If t = $-\frac{1}{2}$ then it is called Randic Index

$$\mathbf{R(G)} = \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{12}} + \frac{2n-1}{2} + \frac{n-2}{4}$$

If we put alkyl or branches of alkyl in space of hydrogen atoms in Cycloalkanes we will get a new chemical graph from Unicyclic , denoted by U_n^{*alkyl} where n is the number of Carbon atoms (see Fig. 5.)

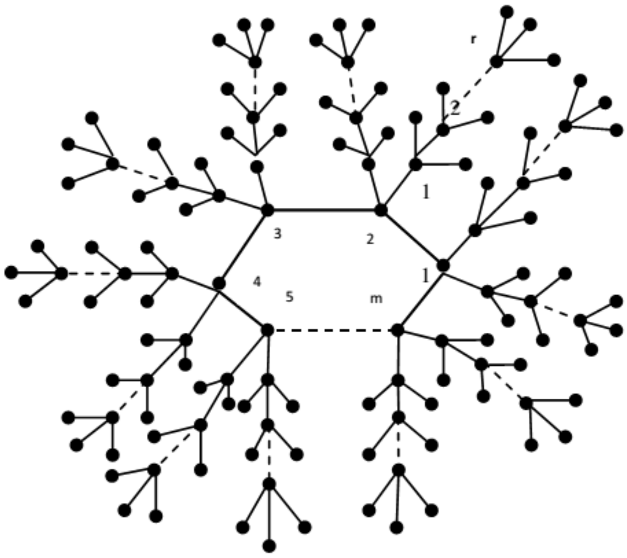

Fig-5. $G = U_n^{*alkyl}$

Theorem 3.4. Let n and r be positive integer numbers, the General Randic Index and the Randic index of a graph G = U_n^{*alkyl} are:-

$$\mathbf{GR}(U_n^{*alkyl}) = (n+2nr)(16)^t + (4nr+2n)(4)^t$$

$$\mathbf{R}(U_n^{*alkyl}) = \frac{n+2nr}{4} + \frac{4nr+2n}{2}$$

Proof:- we have (3n + 6nr) edges. (n + 2nr) edges of them are incidents on a vertex u with $\rho(u) = 4$ and a vertex v with $\rho(v) = 4$, (4nr + 2n) edges of them are incidents on a vertex u with $\rho(u) = 4$ and a vertex v with $\rho(v) = 1$.

Hence by definition of General Randic index we get the following:

$$\mathbf{GR}(U_n^{*alkyl}) = (n+2nr)(16)^t + (4nr+2n)(4)^t$$

If $t = -\frac{1}{2}$ then it is called Randic Index

$$\mathbf{R}(U_n^{*alkyl}) = \frac{n+2nr}{4} + \frac{4nr+2n}{2}$$

CONCLUSIONS

In this paper, we study The Randic and General Randic Indices of Alkanes , cycloalkanes ,the group of Alkyl or branch of alkyl and we study The Randic and General Randic Indices of U_n^{*alkyl} where alkyl or branch of alkyl put in place each hydrogen atom in cycloalkanes .

REFERENCES

1. B. Bollobas, P. Erdos, Graphs of extremal weights, Ars Combin. 50 (1998) 225–233..33.
2. J.Devillers, A.T. Balaban(Eds.), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon and Breach,Amsterdam, 1999.
3. M.V. Diudea, QSPR/QSAR Studies by Molecular Descriptors, Nova Sci. Publ., Huntington, NY, 2000.
4. A.L. Jabir, A. M. Khalaf, E. A. J. AL-Mulla, Hosoya Polynomial of Some Semiconductors, Journal of Kufa For Mathematics and Computer 2 (2), 49-55 (2014).
5. M. Karelson, Molecular Descriptors in QSAR/QSPR, Wily-Interscience, New York, 2000.
6. M. Randic´ , On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975) 6609–6615.
7. R. Todeschini, V. Consonni, Handbook of Molecular Descriptors , Wiley- VCH, Weinheim, 2000.
8. H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc, 69(1947), 17-20.
9. M. Zhang, B. Liu, On a conjecture a bout the Randic index and diameter, MATCH Commun. Math. Comput.Chem. 64 (2010) 433442.
10. R.S. Haoer , K.A. Atan, A. M. Khalaf , R. H asni, Eccentric Connectivity Index Of Unicyclic Graphs With Application To Cycloalkanes, Appl. Math. (2016).
11. R.S. Haoer , K.A. Atan, A. M. Khalaf, M. R. Md. Said, R. Hasni, Eccentric Connectivity Index of Certain Classes of Cycloalkenes, Proceedings of the International Conference on Computing, Mathematics and Statistics (ICMS 2015) Bridging Research Endeavors, Springer, 2017, 235- 242.
12. R.S. Haoer , K.A. Atan, M. R. Md. Said, A. M. Khalaf , R. Hasni, Zagreb-Eccentricity Indices of Unicyclic Graph with application to Cycloalkanes, Journal of Computational and Theoretical Nanoscience 13, 8870-8873 (2016).
13. Mohanad A. Mohammed , K.A. Atan , A. M. Khalaf, M. Rushdan ,R. Hasni, On The Atom Bond Connectivity Index Of Certen Trees and Unicyclic Graphs, Applied Mathematics, (2016).
14. M. A. Mohammed, K. A. Atan, A. M. Khalaf, M. R. Md. Said, and R. Hasni, Atom Bond Connectivity Index of Molecular Graphs of Alkynes and Cycloalkynes, Journal of Computational and Theoretical Nanoscience 13, 6698-6706 (2016).