STUDIA UBB CHEMIA, LIX, 1, 2014 (p. 29-34)
(RECOMMENDED CITATION)

REMARKS ON THE RECIPROCAL DEGREE DISTANCE

LOTFALLAH POURFARAJ[a,*] AND MODJTABA GHORBANI[b]

ABSTRACT. In the present paper we study some properties of a new graph invariant named reciprocal degree distance of some molecular graphs. This new topological index is defined by Hua et al. as $RDD(G) = \sum_{u,v \in E(G)} (d(u) + d(v))[d(u,v)]^{-1}$, where the $d(u,v)$ denotes the distance between vertices u and v.

Key Words: *reciprocal degree distance, graph invariants, octane isomers.*

INTRODUCTION

Theoretical chemistry has many branches. Among them, Mathematical chemistry is an important tool for which applies mathematical methods to predict chemical phenomena without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry for studying molecular structures [1-3]. This theory had an important effect on the development of the chemical sciences [4,5].

Throughout this paper all graphs are simple and connected. We denote the vertex and edge sets of a graph G by $V(G)$ and $E(G)$, respectively. Suppose $\wp$ denotes the class of all graphs. A topological index is a real function $\Lambda: \wp \to \mathbb{R}^+$ by this property that if $G \cong H$ then $\Lambda(G) = \Lambda(H)$. Obviously, the maps $\Lambda_1 = |V(G)|$ and $\Lambda_2 = |E(G)|$ are topological indices. If $x, y \in V(G)$ then the distance $d(x, y)$ between x and y is defined as the length of a minimum path connecting x and y. The Wiener index [6] is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. In other words, the Wiener index is defined as follows:

[a] *Department of Mathematics, Islamic Azad University, Central Tehran Branch (IAUCTB), Tehran, I.R. Iran*
[b] *Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran,* 16785 – 136, *I.R. Iran*
* *Corresponding author: l.pourfaraj@iauctb.ac.ir*

$$W(G) = \frac{1}{2}\sum_{x,y\in V(G)} d(x,y).$$

The reciprocal degree distance $RDD(G)$ of a molecular graph G was proposed by Hua and Zhang [7] as

$$RDD(G) = \sum_{u,v\in V(G)} (d(u)+d(v))\frac{1}{d(u,v)},$$

where $d(u)$ denotes the degree of the vertex u in G. The eccentricity of a vertex u is also defined as $\varepsilon(u) = Max\{d(x,u) \mid x \in V(G)\}$. The maximum eccentricity over all vertices of G is called the diameter of G and denoted by $d(G)$ and the minimum eccentricity among the vertices of G is called radius of G and denoted by $r(G)$.

The Harary index $H(G)$ of a graph G on n vertices is based on the concept of reciprocal distance and is defined the half-sum of the off-diagonal elements of the reciprocal distance matrix $RD(G)$:

$$H(G) = \frac{1}{2}\sum_{uv\in V(G)} \frac{1}{d(u,v)},$$

where the ij-th entry of reciprocal distance matrix $RD(G)$ is

$$RD(G)_{ij} = \frac{1}{d(v_i,v_j)}.$$

Here, our notations are standard and mainly taken from standard book of graph theory such as [8] as well as [9 – 13].

RESULTS AND DISCUSSION

In this section we compute some bounds of reciprocal degree distance of graphs. The following theorem presents a sharp bound of reciprocal degree distance. Here, the complete graph and a star graph on n vertices are denoted by K_n and S_n, respectively.

Example 1.

$RDD(K_n) = n(n-1)^2$ and $RDD(S_n) = n(3n+1)/2$.

In generally, for regular graph we have:

Lemma 1. Let G be a regular graph of degree r, then

$$RDD(G) = 4r \times H(G).$$

Vertex Transitive Graphs

A bijection σ on vertices set of graph G is named an automorphism of graph, if it preserves the edge set. In other word, σ is an automorphism if for every edge $e = uv$ of E then $\sigma(e)=\sigma(u)\sigma(v)$ be an edge of E. Let $Aut(G) = \{\alpha : V \to V, \alpha$ is bijection$\}$, then $Aut(G)$ under the composition of mappings forms a group. $Aut(G)$ acts transitively on V if for any vertices u and v in V there is $\alpha \in Aut(G)$ such that $\alpha(u) = v$. For given vertex u, let

$$T(u) = \sum_{v \in V(G)} d(u,v)^{-1}.$$

Then we have the following Lemma:

Lemma 2. If G be a vertex transitive graph, then for any pair of vertices such as u and v, $T(u) = T(v)$.

Proof. Since G is vertex transitive, so there is an automorphism α in $Aut(G)$ such that $\alpha(u) = v$. Hence,

$$T(v) = \sum_{x \in V(G)} \frac{1}{d(x,v)} = \sum_{x \in V(G)} \frac{1}{d(x,\alpha(u))}$$

$$= \sum_{y \in V(G)} \frac{1}{d(\alpha(y),\alpha(u))} = \sum_{y \in V(G)} \frac{1}{d(y,u)} = T(u).$$

Theorem 3. If G be a vertex transitive graph on n vertices, then for a given vertex u,

$$RDD(G) = 2nrT(u).$$

Proof. Since G is vertex transitive graph, G is regular. So the reciprocal degree distance is:

$$RDD(G) = \sum_{u,v \in V(G)} (d(u) + d(v)) \frac{1}{d(u,v)} = 2r \times \sum_{u,v \in V(G)} \frac{1}{d(u,v)}$$

$$= 2r \times \sum_{u \in V(G)} T(u) = 2nrT(u).$$

As a result of Theorem 3, we compute reciprocal degree distance of well-known fullerene namely C_{60}, see Figure 1.

The graph of this fullerene is a three connected cubic graph whose faces are pentagons and hexagons. One can prove easily by Euler's theorem that numbers of pentagonal and hexagonal faces are 12 and 20, respectively. This fullerene is the only vertex transitive IPR (Isolated Pentagonal Rule) fullerene. The smallest fullerene is dodecahedron C_{20} and it is composed of exactly 12 pentagons. In other word, C_{20} is the only fullerene without any hexagonal faces. The fullerene C_{20} is non-IPR vertex transitive. By a direct computation we get for every vertex u, $T(u)$ =179/20. Hence, by using Theorem 4 $RDD(C_{20})$ = 1074. By using a similar way for the fullerene C_{60}, for any vertex u in $V(C_{60})$, $T(u)$ = 4259/168 and thus $RDD(C_{60})$ =63885/7.

Figure 1. 3-*D* graph of fullerene C_{60}.

A hypercube (Figure 2) is a regular graph, where its vertex set consisted of all *n*-tuples $b_1b_2\ldots b_n$ with $b_i \in \{0,1\}$ and Two vertices are adjacent if and only if the corresponding tuples differ in precisely one place. Darafsheh in [14] proved that hypercube is a vertex transitive graph of order *n* and hence by using Theorem 3, we have:

Theorem 4. $RDD(H_n) = 2^{n+2} - 2(n+1)$.

Proof. The number of vertices of a hypercube H_n is 2^n and the number of pair of vertices at distance *i* is $C(n,i) = \frac{n!}{i!(n-i)!}$. This implies that for every vertex *u*, $T(u) = \sum_{i=1}^{n} C(n,i)/i = (2^{n+1} - n - 1)/n$. Since every vertex has degree *n*, by using Theorem 3 the proof is completed.

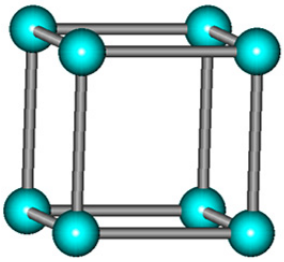

Figure 2. 3-D graph of a hypercube, where *n* = 3.

RECIPROCAL DEGREE DISTANCE OF OCTANE ISOMERS

The aim of this section is to compute the reciprocal degree distance of octane isomers. Then we obtain a good linear correlation between *RDD,* acentric factor and entropy(*S*) of the octane isomers, *e.g.* R^2 = 0.9726. These values are reported in Table 1. All isomers of octane are depicted in Figure 3.

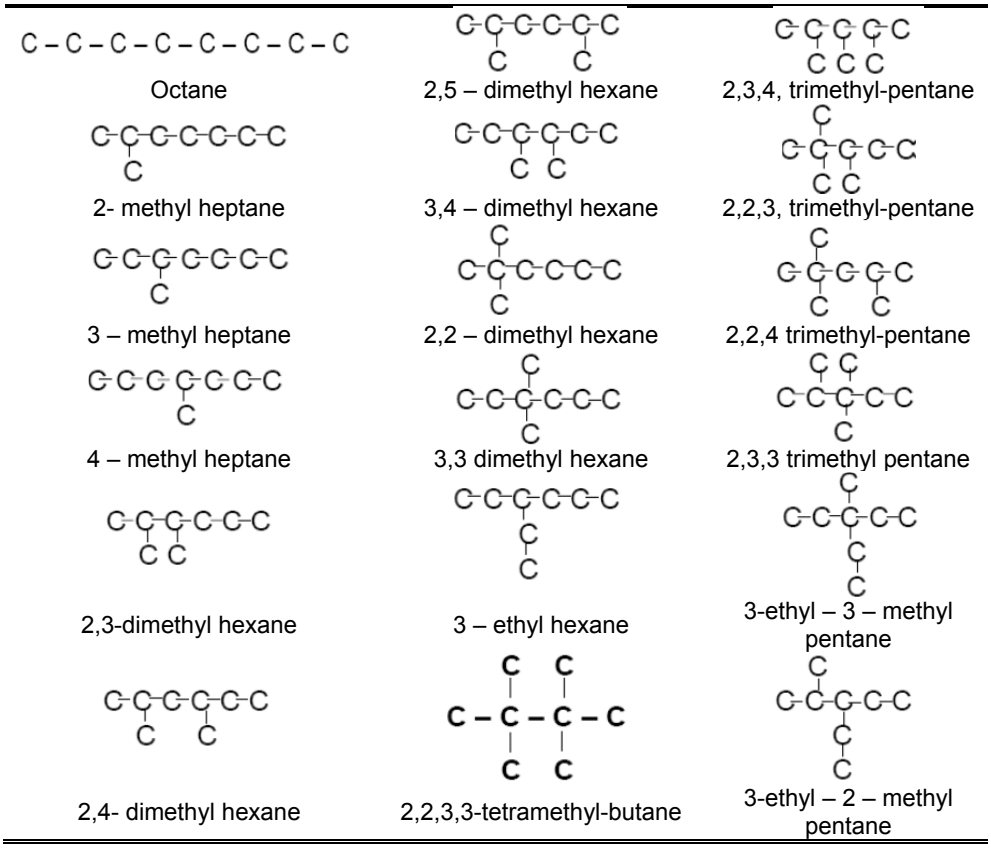

Figure 3. All octane isomers.

Table 1. Acen Fac, *S* and *RRD* of the octane isomers.

Molecule	**Acent Fac**	***S***	***RRD***
octane	0.397898	111	99.57
2-methy l-heptane	0.377 916	109.84	104.33
3-methyl-heptane	0.371002	111.26	106.2
4-methyl-heptane	0.371504	109.32	112.27
3-ethyl-hexane	0.362472	109 .43	108.6
2 ,2-dimethyl-hexane	0.339426	103.42	113.4
2 ,3-dimethyl-hexane	0.348247	108.02	112.27
2 ,4-dimethyl-hexane	0.344 223	106.98	112.27
2 ,5-dimethyl-hexane	0.35683	105.72	109.2
3 ,3-dimethyl-hexane	0.322596	104.74	116.47
3 ,4-dimethyl-hexane	0.340 345	106.59	113.8
2-methyl-3-ethyl-pentane	0.332433	106.06	114.33
3-methyl-3-ethyl-pentane	0.306 899	101.48	119
2 ,2 ,3-trimethyl-pentane	0.300816	101.31	121.67

Molecule	Acent Fac	*S*	*RRD*
2 ,2 ,4-trimethyl-pentane	0.30537	104.09	118.67
2 ,3 ,3-trimethyl-pentane	0.293 177	102.06	122.67
2,3 ,4-trimethyl-pentane	0.317422	102.39	118
2,2,3,3-tetramethylbutane	0.255294	93.06	130

CONCLUSION

Topological descriptors are very important tools in chemical graph theory. Among them topological indices play a fundamental role in predicting chemical phenomena. The reciprocal degree distance is a topological index was defined by Hua and Zhang. In this paper reciprocal degree distance of some vertex transitive chemical graphs were computed.

ACKNOWLEDGMENTS

The results in this paper are part of “On The Reciprocal Degree Distance Of Graphs” project. Support of this work was provided for L. Pourfaraj and M. Ghorbani by grant from Islamic Azad University, Central Tehran Branch, Tehran. Iran. Also the authors would like to thank Islamic Azad University, Central Tehran Branch, Tehran. Iran.

REFERENCES

1. M.V. Diudea, (Ed.), *QSPR/QSAR Studies by Molecular Descriptors*, NOVA, New York, **2001**.
2. M.V. Diudea, I. Gutman, L. Jäntschi, *Molecular Topology*, NOVA, New York, **2002**.
3. M.V. Diudea, M.S. Florescu, P. V. Khadikar, *Molecular Topology and Its Applications*, EFICON, Bucharest, **2006**.
4. I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer - Verlag, New York, **1986**.
5. M.A. Johnson, G.M. Maggiora, *Concepts and Applications of Molecular Similarity*, Wiley Interscience, New York, **1990**.
6. H. Wiener, *J. Am. Chem. Soc*., **1947**, *69*, 17.
7. H. Huaa, S. Zhang, *Discrete Appl. Math*., **2012**, *160*, 1152.
8. S. Gupta, M. Singh, A.K. Madan, *J. Math. Anal. Appl*., **2002**, *275*, 386.
9. N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, FL, **1992**.
10. S. Sardana, A.K. Madan*, MATCH Commun. Math. Comput. Chem*., **2001**, *43*, 85.
11. A.R. Ashrafi, M. Saheli, M. Ghorbani, *Journal of Computational and Applied Mathematics*, **2011**, *235*, 4561.
12. M. Jalali, M. Ghorbani, *Studia UBB Chemia,* **2009**, *4(2),* 145.
13. I. Gutman, N. Trinajstić, *Chem. Phys. Lett*., **1972**, *17*, 535.
14. M.R. Darafsheh, *Acta. Appl. Math*., **2010**, *110*, 1225.