ISSN (Online): 2456-5717

International Journal of Advanced Research in Basic Engineering Sciences and Technology (IJARBEST)
Vol.4 Issue.3 March 2018

On Degree-Distance Index of Hexagonal Network

S. Prabhu[1] G. Murugan[2*] Natarajan Muthuraman[3]

[1]Department of Applied Mathematics, Sri Venkateswara College of Engineering, Sriperumbudur, India.
[2]Department of Mathematics, Chendu College of Engineering and Technology, Madurantakam, India.
[3]Department of Computer Science Engineering, Sri Venkateswara College of Engineering, Sriperumbudur, India.

Abstract: **Topological index is a numeric quantity associated with the molecular graph of the chemical compound. There are different types of topological indices in the literature which are mainly categorized into degree-based and distance-based topological indices. These topological indices correlate boiling point, stability, strain energy and other physic-chemical properties of chemical compounds. Wiener index is an ancient topological index which is introduced by Harold Wiener while he was working on steaming point of paraffin. The convex partition method and extended convex partition method accommodates the problem of finding Wiener index of large family of molecular graphs. As these methods are not universe, we have some of the molecular graphs for which these methods are not feasible. In particular name a few we have TiO_2 nanotube, Boron and alpha-boron nanotubes and networks like hexagonal network. In this paper we find the Wiener, Gutman and Degree distance index for hexagonal network using computer algorithm and programme.**

Keywords: **Molecular graphs, Graph invariants, hexagonal networks, topological indices, Wiener index, Degree-distance index, Gutman index.**

I. Introduction

The structure of a chemical composite can be symbolized by a graph whose vertex and edge identify the atom and bonds respectively. Computational drug design is a rapidly growing field and a very important domain in the discipline of medicinal chemistry. International Union of Pure and Applied Chemistry (IUPAC), Medicinal Chemistry Section Committee has pointed out the topological index as one among the important terms used in computational drug design for easy reference purposes [28]. Topological index is the numeric quantity of molecule that is mathematically derived from the structural graph of a molecule. The topological indices are used in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) studies.

Let $V(G)$ and $E(G)$ be respectively denotes the set of all vertices and set of all edges of a molecular graph G. The cardinality of these sets represents the number of vertices and edges. An edge in $E(G)$ is represented by $e = uv$ with end vertices u and v (u and v are adjacent). Throughout this paper $d(u,v)$ represents the distance (No. of edges) between u and v. The diameter of the graph G is defined by $diam(G) = Max\{d(u,v) : u,v \in V(G)\}$ and $d_G(u)$ is the degree (the number of vertices adjacent to u or the number of edges incident with u) of the vertex u in G.

The first idea of this index originated from the effort ended by H. Wiener in 1947 while he was working on steaming limit of paraffin [29] and this is the first topological index in the field of computational and mathematical chemistry. The Wiener index of the graph G is defined as [15]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

For details on Wiener index consult paper [14, 8, 9].

In the past few decades, an enormous quantity of mathematical investigations were stated on graph invariants instigating from chemistry. For applications of these graph invariants, the research community can refer the chemical literature [6, 7, 10, 25].

The graph invariants (Topological indices) are based on vertex degrees and the distances between vertices. Most of the degree based topological indices were computed by direct computation and edge partition methods whereas the distance based topological indices like Wiener [18], vertex Szeged index [13], edge Szeged index [30], edge–vertex Szeged index [20], and total Szeged [20] are computed using convex partition method [18]. The extension of this method is given by Arockiaraj et al. in [1]. In this paper we compute the Wiener, Gutman and degree distance index of hexagonal network.

The degree distance was first given by Dobrynin and Kochetova in [11] and by Gutman [12], who used other name Schultz molecular topological index. The degree distance of a vertex $x \in V(G)$ is defined and denoted by

$$D'(x) = d(x) \sum_{y \in V(G)} d(x,y)$$

$$D'(G) = \sum_{x \in V(G)} D'(x)$$

Yet another way of defining the same invariant is the following

$$DD(G) = \sum_{\{x,y\} \subseteq V(G)} d(x)d(y)d(x,y)$$

In the literature Degree distance index of a graph is investigated by many people. The unique extremal graph for minimum $DD(G)$ is given in [21]. This result solves the conjecture posted by Dobrynin and Kochetova [11]. The are several properties on degree distance of a connected graph of given order and size were presented in [2, 21, 23]. The two extremal values of degree distance of a unicyclic graph were discussed in [3, 16, 17, 22]. An ordering of connected graphs with respect to degree distance were given in [24, 26]. Dankelmann et al. [5] solved the conjecture on degree distance of a graph posted by Tomescu [21]. The reverse degree distance is also reported in [31].

II. Results and Discussion

Hexagonal networks are applied in chemistry to model benzenoid hydrocarbons [27]. Hexagonal networks are the partition of a plane into equilateral triangles. These networks are based on regular triangular tessellations studied in [4]. It also has application in computer graphics and image processing [19]. A hexagonal network $HX(n)$ of dimension n has $3n^2 - 3n + 1$ vertices and $9n^2 - 15n + 6$ edges, where n is the number of vertices on one side of the hexagon [4]. The vertex set of $HX(n)$ is $V\big(HX(n)\big) = \{(\alpha,\beta,\gamma)\colon -n \le \alpha,\beta,\gamma \le n\}$. The diameter of $HX(n)$ is $2n-2$ and vertex partition is given in Table 1. There is exactly one vertex at distance $n - 1$ from each of the corner vertices (3-degree vertices). This vertex is called the centre of $HX(n)$ and denoted by $(0,0,0)$. See Figure 1.

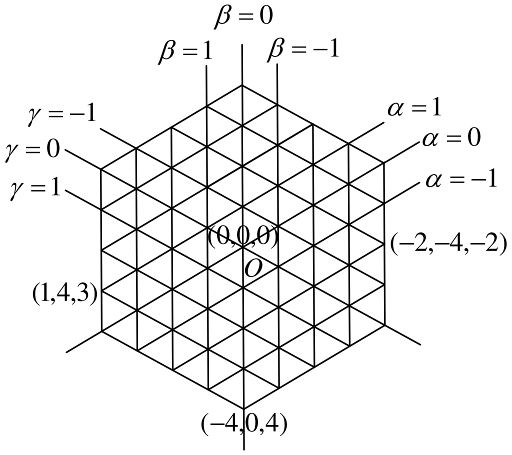

Fig 1: Co-ordinate axis in $HX(n)$

Table 1: Vertex of Partition of $HX(n)$

S. No	Vertex Partition	$\lvert V_i\rvert$
1	$V_1 = \{u\colon d_G(u) = 3\}$	6
2	$V_2 = \{u\colon d_G(u) = 4\}$	$6(n-2)$
3	$V_3 = \{u\colon d_G(u) = 6\}$	$3n^2 - 9n + 7$

Observation 1.1: Let (α,β,γ) be any vertex of $HX(n)$. Then $\overline{(\alpha,\beta,\gamma)}$ is also a vertex of $HX(n)$ where $\overline{(\alpha,\beta,\gamma)} = (-\alpha,-\beta,-\gamma)$.

Observation 1.1: Let V_1 be the set of all three degree vertices of $HX(n)$ and $(\alpha,\beta,\gamma) \in V_1$. Then V_1 satisfies the following conditions

(i) $|\alpha| + |\beta| + |\gamma| = 2n$
(ii) $\alpha + \beta \neq 0\ ;\beta + \gamma \neq 0$
(iii) $\alpha \neq \beta \neq \gamma$
(iv) $\alpha = 0$ or $\beta = 0$ or $\gamma = 0$

Observation 1.3: Let V_2 be the set of all four degree vertices of $HX(n)$ and $(\alpha,\beta,\gamma) \in V_2$. Then V_2 satisfies the following conditions

(i) $|\alpha| + |\beta| + |\gamma| = 2n$
(ii) $\alpha \neq \beta \neq \gamma$
(iii) $|\alpha| + |\beta| = |\gamma|$; $|\beta| + |\gamma| = |\alpha|$; $|\alpha| + |\gamma| = |\beta|$

Lemma 1.1:

Let G be a $HX(n)$ and $u = (l_1, m_1, n_1)$ and $v = (l_2, m_2, n_2)$ be any two vertices of G. Then $d_G(u, v) = \frac{1}{2}[|l_1 - l_2|+|m_1 - m_2|+|n_1 - n_2|]$

The proof of the above lemma is trivial from the addressing scheme presented in the Figure 1. Using this result as a key we compute the wiener, Gutman and degree distance index of hexagonal network using computer program.

C++ Program

For every positive integer $n \geq 1$, the Wiener index, Gutman index, Degree distance index and ratio between them for $HX(n)$ is computed by using following C++ Program:

```
#include<stdio.h>
#include<math.h>
main()
{
        int
a[100000][3],b[10][3],c[10000][3],d[10000][3],n,i,j,k,x,y,f,q,w,e,z,l[3],m[3],p,r=0,s=0,t=0,h=0,g=0,flag=
0,flag1=0,flag2=0,flag3=0,flag4=0;
        float i0,i1,i2,i3,i4,i5,i6,j1,j2,j3,j4,j5,j6;
        unsigned long long int dsum=0,gsum=0,wsum=0;
        printf("Enter the HX value:");
        scanf("%d",&n);
        f=(3*n*n)-(3*n)+1;
        printf("Total number of points:%d\n",f);
        n--;
        x=n;
        y=0;
        i0=(float) 1/2;
        i1=(float) 9/2;
        i2=(float) 16/2;
        i3=(float) 36/2;
        i4=(float) 12/2;
        i5=(float) 18/2;
        i6=(float) 24/2;
        j1=(float) 6/2;
        j2=(float) 8/2;
        j3=(float) 12/2;
        j4=(float) 7/2;
        j5=(float) 9/2;
        j6=(float) 10/2;
        for(j=n;j>=0;j--)
        {
                for(i=x,k=y;i>=y,k<=x;i--,k++)
                {
                        h=0;
                        a[g][h]=i;
                        h++;
                        a[g][h]=j;
                        h++;
                        a[g][h]=k;
                        h++;
                        g++;
                }
        y--;
    }
    for(i=0,j=f-1;i<f/2,j>f/2;i++,j--)
    {
        for(k=0;k<3;k++)
        {
            a[j][k]=-a[i][k];
        }
    }

    for(i=0;i<f;i++)
    {
        j=0;
        q=abs(a[i][j]);
        w=abs(a[i][j+1]);
        e=abs(a[i][j+2]);
        if((q+w+e==2*n)&&(q==0||w==0||e==0))
        {
            for(j=0;j<3;j++)
            {
                b[r][j]=a[i][j];
            }
            r++;
            flag1++;
        }
        else if(q+w+e==2*n)
        {
            for(j=0;j<3;j++)
            {
                c[s][j]=a[i][j];
            }
            s++;
            flag2++;
        }
        else
        {
            for(j=0;j<3;j++)
            {
                d[t][j]=a[i][j];
            }
            t++;
            flag3++;
        }
    }

    printf("\n\n3 degree vertex:\n");
    for(i=0;i<flag1;i++)
    {
        for(j=0;j<3;j++)
        {
            printf("%d ",b[i][j]);
        }
        printf("\n");
        flag++;
    }
    printf("3 degree vertex Experimented value:%d",flag1);
    printf("\n\n4 degree vertex:\n");
    for(i=0;i<flag2;i++)
```

```
{
        for(j=0;j<3;j++)
        {
                printf("%d ",c[i][j]);
        }
        printf("\n");
        flag++;
}
printf("4 degree vertex Experimented value:%d",flag2);
printf("\n\n6 degree vertex:\n");
for(i=0;i<flag3;i++)
{
        for(j=0;j<3;j++)
        {
                printf("%d ",d[i][j]);
        }
        printf("\n");
        flag++;
}
printf("6 degree vertex Experimented value:%d",flag3);
printf("\n\nTotal Experimented value:%d",flag);

for(i=0;i<flag1-1;i++)
{
        for(j=i+1;j<flag1;j++)
        {
                p=0;
                for(k=0;k<3;k++)
                {
                        l[k]=b[i][k];
                        m[k]=b[j][k];
                        p+=abs(l[k]-m[k]);
                }
                gsum+=p*i1;
                wsum+=p*i0;
                dsum+=p*j1;
                flag4++;
        }
}

for(i=0;i<flag2-1;i++)
{
        for(j=i+1;j<flag2;j++)
        {
                p=0;
                for(k=0;k<3;k++)
                {
                        l[k]=c[i][k];
                        m[k]=c[j][k];
                        p+=abs(l[k]-m[k]);
                }
                gsum+=p*i2;
                wsum+=p*i0;
                dsum+=p*j2;
                flag4++;
        }
}
```

```
for(i=0;i<flag3-1;i++)
{
        for(j=i+1;j<flag3;j++)
        {
                p=0;
                for(k=0;k<3;k++)
                {
                        l[k]=d[i][k];
                        m[k]=d[j][k];
                        p+=abs(l[k]-m[k]);
                }
                gsum+=p*i3;
                wsum+=p*i0;
                dsum+=p*j3;
                flag4++;
        }
}

for(i=0;i<flag1;i++)
{
        for(j=0;j<flag2;j++)
        {
                p=0;
                for(k=0;k<3;k++)
                {
                        l[k]=b[i][k];
                        m[k]=c[j][k];
                        p+=abs(l[k]-m[k]);
                }
                gsum+=p*i4;
                wsum+=p*i0;
                dsum+=p*j4;
                flag4++;
        }
}

for(i=0;i<flag1;i++)
{
        for(j=0;j<flag3;j++)
        {
                p=0;
                for(k=0;k<3;k++)
                {
                        l[k]=b[i][k];
                        m[k]=d[j][k];
                        p+=abs(l[k]-m[k]);
                }
                gsum+=p*i5;
                wsum+=p*i0;
                dsum+=p*j5;
                flag4++;
        }
}


for(i=0;i<flag2;i++)
{
        for(j=0;j<flag3;j++)
```

```
                {
                        p=0;
                        for(k=0;k<3;k++)
                        {
                                l[k]=c[i][k];
                                m[k]=d[j][k];
                                p+=abs(l[k]-m[k]);
                        }
                        gsum+=p*i6;
                        wsum+=p*i0;
                        dsum+=p*j6;
                        flag4++;
                }
        }
        printf("\n%dC2:%d",f,flag4);
        printf("\nWeiner Sum:%llu",wsum);
        printf("\nGutmann Sum:%llu",gsum);
        printf("\nDegree Distance Sum:%llu",dsum);
        printf("\n3 degree vertex Experimented value:%d",flag1);
        printf("\n4 degree vertex Experimented value:%d",flag2);
        printf("\n6 degree vertex Experimented value:%d",flag3);
        printf("\nTotal Experimented value:%d",flag);
}
---------------------------------------------------------------------------------------------
```

Output:

n	$\|V_1\|$	$\|V_2\|$	$\|V_3\|$	$\|V(G)\|$	$W(G)$	$Gut(G)$	$D'(G)$
2	6	0	1	7	30	324	198
3	6	6	7	19	396	7080	3360
4	6	12	19	37	2142	47100	20130
5	6	18	37	61	7542	185592	74928
6	6	24	61	91	20592	543852	211854
7	6	30	91	127	47502	1316976	500592
8	6	36	127	169	97188	2791572	1042314
9	6	42	169	217	181764	5363472	1975584
10	6	48	217	271	317034	9555444	3482262
11	6	54	271	331	522984	16034904	5793408
12	6	60	331	397	824274	25631628	9195186
13	6	66	397	469	1250730	39355464	14034768
14	6	72	469	547	1837836	58413912	20726238
15	6	78	547	631	2627226	84230704	29756560
16	6	84	631	721	3667176	118455216	41691208
17	6	90	721	817	5013096	162996512	57181720
18	6	96	817	919	6728022	220057344	76964528
19	6	102	919	1027	8883108	292052352	101892336
20	6	108	1027	1141	11558118	381793728	132880784
21	6	114	1141	1261	14841918	492293504	171003056
22	6	120	1261	1387	18832532	627051648	217405104
23	6	126	1387	1519	23639336	789819904	273365344
24	6	132	1519	1657	29371868	984828416	340307808
25	6	138	1657	1801	36182976	1216605056	419730272
26	6	144	1801	1951	44189216	1490128512	513282272
27	6	150	1951	2107	53564488	1810358144	623003008
28	6	156	2107	2269	64466064	2183537664	750730496
29	6	162	2269	2437	77080048	2617854976	898445312

30	6	168	2437	2611	91576176	3118729216	1068558976
31	6	174	2611	2791	108161696	3692178432	1262941696
32	6	180	2791	2977	127117216	4347153408	1486075008
33	6	186	2977	3169	148652544	5084992512	1739878144
34	6	192	3169	3367	172907872	5920211456	2026412928
35	6	198	3367	3571	200386848	6861762048	2347900160
36	6	204	3571	3781	231034784	7925750272	2709995776
37	6	210	3781	3997	265343904	9107546112	3115038208
38	6	216	3997	4219	304018624	10438281216	3572114432
39	6	222	4219	4447	345913152	11933955072	4079330048
40	6	228	4447	4681	393166592	13562846208	4621854208
41	6	234	4681	4921	444818560	15389589504	5205032448
42	6	240	4921	5167	502000640	17430755328	5895647744
43	6	246	5167	5419	566709888	19558567936	6657934848
44	6	252	5419	5677	629338368	21958684672	7495272448
45	6	258	5677	5941	699884288	24706453504	8405850624
46	6	264	5941	6211	784784512	27665117184	9407028224
47	6	270	6211	6487	878448384	30893588480	10133841920
48	6	276	6487	6769	978892032	34370441216	11117538304
49	6	282	6769	7057	1085469696	35253702656	12358457344
50	6	288	7057	7351	1179087360	37363912704	13783692288
60	6	348	10267	10621	2147483648	68790517760	22356957184
70	6	408	14077	14491	2296282112	86263267328	34359738368
80	6	468	18487	18961	4041338368	137438953472	34359738368
90	6	528	23497	24031	4294967296	137438953472	35576950784
100	6	588	29107	29701	4294967296	137438953472	68719476736

REFERENCES

[1] M.Arockiaraj and A.J. Shalini, Extended Cut Method for Edge Wiener, Schultz and Gutman Indices with Applications, MATCH Commun. Math. Comput. Chem. 76 (2016) 233-250.

[2] O.Bucicovski and S.M. Cioaba, The minimum degree distance of graphs of given order and size. Discrete Appl. Math. 156 (2008), 3518–3521.

[3] A.Chen, Ordering unicyclic graphs by their degree distance. J. of Fuzhou Univ. Nat. Sci. 32, 664–668 (2004).

[4] M.S. Chen, K. G. Shin, D. D. Kandlur, Addressing, routing and broadcasting in hexagonal mesh multiprocessors, IEEE Transactions on Computers Vol. 39, 10-18 (1990).

[5] P.Dankelmann, I. Gutman, S. Mukwembi and H.C. Swart, On the degree distance of a graph. Discrete Appl. Math. 157 (2009), 2773–2777.

[6] J. Devillers and A.T. Balaban (Eds.), Topological Indices and Related Descriptors in QSAR and QSPR. Gordon and Breach, Amsterdam, 1999.

[7] M.V.Diudea, I. Gutman and L. Jantschi, Molecular Topology. Nova, New York, 2001.

[8] A.A.Dobrynin, R. Entringer, I. Gutman, Wiener index of Trees: Theory and applications, Acta Appl. Math. 66 (2001) 211–249.

[9] A.A.Dobrynin, I. Gutman, S. Klavzar, P. Zigert, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–294.

[10] Gutman and B. Furtula (Eds.), Novel Molecular Structure Descriptors -Theory and Applications. I-II, Univ. Kragujevac, Kragujevac, 2010.

[11] A.A.Dobrynin and A.A. Kochetova, Degree distance of a graph: a degree analogue of the Wiener index. J. Chem. Inf. Comput. Sci. 34 (1994), 1081-1086.

[12] Gutman, Selected properties of the Schultz molecular topological index. J. Chem. Inf. Comput. Sci. 34 (1994), 1087-1089

[13] Gutman, I.; Klavzar, S., An Algorithm for the Calculation of the Szeged Index of Benzenoid Hydrocarbons, J. Chem. Inf. Comput. Sci., 35 (1995) 1011-1014.

[14] I.Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer–Verlag, Berlin 1986.

[15] H.Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, Bull. Chem. Soc. Japan 44 (1971) 2332–2339.

[16] Y.Hou and A. Chang, The unicyclic graphs with maximum degree distance. J. Math. Study 39 (2006), 18–24.

[17] A.Ilic, D. Stevanovic, L. Feng, G. Yu and P. Dankelmann, Degree distance of unicyclic and bicyclic graphs. Discrete Appl. Math. 159 (2011), 779–788.

[18] Klavzar, S.; Gutman, I.; Mohar, B., Labeling of Benzenoid Systems which Reflects the Vertex-Distance Relations *J.* Chem. Inf. Comput. Sci., 35(3) (1995) 590-593.

[19] E.Kranakis, H. Singh and J. Urrutia, Compass routing in geometric graphs, Proceedings of the 11th Canadian Conference on Computational Geometry, (CCCG-99), (1999), 51-54.

[20] Manuel, P.; Rajasingh, I.; Arockiaraj, M. Total-Szeged Index of C_4-Nanotubes, C_4-Nanotori and Dendrimer Nanostars, J. Comput. Theor. Nanosci., 10 (2013) 405-411.

[21] Tomescu, Some extremal properties of the degree distance of a graph. Discrete Appl. Math. 98 (1999), 159–163.

[22] A.I. Tomescu, Unicyclic and bicyclic graphs having minimum degree distance. Discrete Appl. Math. 156 (2008) 125–130.

[23] Tomescu, Properties of connected graphs having minimum degree distance. Discrete Math. 309 (2009) 2745–2748.

[24] Tomescu, Ordering connected graphs having small degree distances. Discrete Appl. Math. 158 (2010) 1714–1717.

[25] R. Todeschini and V. Consonni, Molecular Descriptors for Chemoinformatics. Wiley- VCH, Weinheim, 2009.

[26] Tomescu and S. Kanwal, Ordering connected graphs having small degree distances. II. MATCH Commun. Math. Comput. Chem. 67 (2012), 425–437.

[27] R. Tosic, D. Masulovic, I. Stojmenovic, J. Brunvoll, B.N. Cyvin, and S.J. Cyvin, Enumeration of polyhex hydrocarbons to h = 17, Journal of Chemical Information and Computer Sciences, 35, (1995) 181-187.

[28] H.Van De Waterbeemd, R. E. Carter, G. Grassy, H. Kubinyi, Y. C. Martin, M. S. Tute, P. Willett, Glossary of terms used in Computational Drug Design, Pure & Appl. Chem., 69(5) (1997) 1137-1152.

[29] H.Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69 (1947) 17–20.

[30] Yousefi-Azari, H.; Khalifeh, M. H.; Ashrafi, A. R., Calculating the edge Wiener and edge Szeged indices of graphs, J. Comput. Appl. Math., 235 (2011) 4866-4870.

[31] B.Zhou and N. Trinajstic, On reverse degree distance. J. Math. Chem. 47 (2010), 268–275.