# ON NEIGHBORHOOD DEGREE DISTANCE AND NEIGHBORHOOD GUTMAN INDEX OF MOLECULAR GRAPHS

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**Abstract**

Let $G = (V, E)$ be a molecular graph with $|V| = n$ and $|E| = m$. In search of novel topological indices with high predicting power of physic-chemical properties of chemical compounds, we have conceived the neighborhood degree distance index and neighborhood Gutman index. In this paper, the QSPR study carried on set of octane isomers and surprisingly these two parameters shows good correlation to various physic-chemical properties of octane isomers compared with other classical distance parameters. Further, we obtain the formulae for various transformation graphs.

## 1 Introduction

Let $G$ be a simple graph. The order of a graph is $|V(G)|$, its number of vertices denoted by $n$. The size of a graph is $|E(G)|$, its number of edges denoted by $m$. The degree of a vertex $v$, denoted by $d_G(v)$. The subdivision graph $S_1(G)$ is the graph attained from $G$ by replacing each of its edges by a path of length 2. The line graph $L(G)$ of a graph is the graph derived from $G$ in such a way that the edges in $G$ are replaced by vertices in $L(G)$ and two vertices in $L(G)$ are connected whenever the corresponding edges in $G$ are adjacent [8]. For any number $d$, we define $V_d = \{u \in V(G) \backslash s_G(u) = d\}$, in which $s_G(u) = \sum_{v \in N_G(u)} d_G(v)$ and $N_G(u) = \{v \in V(G) \backslash uv \in E(G)\}$.

Topological indices are numerical parameters of a graph which are invariant under graph isomorphisms. Nowadays, there are many such indices that have found applications in Mathematical Chemistry especially in the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) [12–14]. A large number of such indices depend only on the distance between the unordered pair of vertices of molecular graph. One of them is the Wiener index, which is named after H. Wiener [15] and is defined as:

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} d_G(u, v). \tag{1}$$

Later, several degree and distance based topological indices have been studied extensively by the researchers. To list few of them such as terminal Wiener index $TW(G)$ [5], degree-distance index$DD(G)$ [3], Gutman index$GI(G)$ [7] and Ashwini index$\mathcal{A}(G)$ [11] of molecular graphs, which are defined as follows:

$$TW(G) = \sum_{\{u,v\subseteq V_T(G)\}} d(u, v \setminus G) = \sum_{1\leq i<j\leq k} d(u, v \setminus G)$$

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v)[deg_G(u) + deg_G(v)]. \tag{2}$$

$$GI(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v)[deg_G(u)deg_G(v)]. \tag{3}$$

$$\mathcal{A}(T) = \sum_{1\leq i<j\leq n} d_{_T}(v_i, v_j)[deg_{_T}(N(u_i)) + deg_{_T}(N(v_j))]. \tag{4}$$

Where $N(v) = \{u \in V(G) \colon uv \in E(G)\}$.

Motivated by the previous research on topological descriptors and their applications, we now define two novel topological indices for of a molecular graph $G$ as follows:

$$NDD(G) = \sum_{1\leq i<j\leq n} d_{_G}(v_i, v_j)[deg_{_G}(N(u_i)) + deg_{_G}(N(v_j))] \tag{5}$$

$$NGI(G) = \sum_{1\leq i<j\leq n} d_{_G}(v_i, v_j)[deg_{_G}(N(u_i)) \times deg_{_G}(N(v_j))] \tag{6}$$

Where $N(v) = \{u \in V(G) \colon uv \in E(G)\}$.

## 2 On chemical applicability of the $NDD$-index and $NGI$-index

Here we have examined the chemical applicability of the $NDD$-index and $NGI$-index and compared the values of $NDD$-index and $NGI$-index for modeling the physical properties [boiling points(BP), molar volumes (mv) at 20°C, molar refractions (mr) at 20°C, heats of vaporization (hv) at 25°C, surface tensions (st) 20°C and melting points (mp), acentric factor (AcentFac) and DHVAP] of octane isomers. The $\mathcal{RS}(G)$ was tested using a data set of octane isomers found at [15]. The values are compiled in Table 1.

**Table 1**- Physico-chemical properties of octane isomers

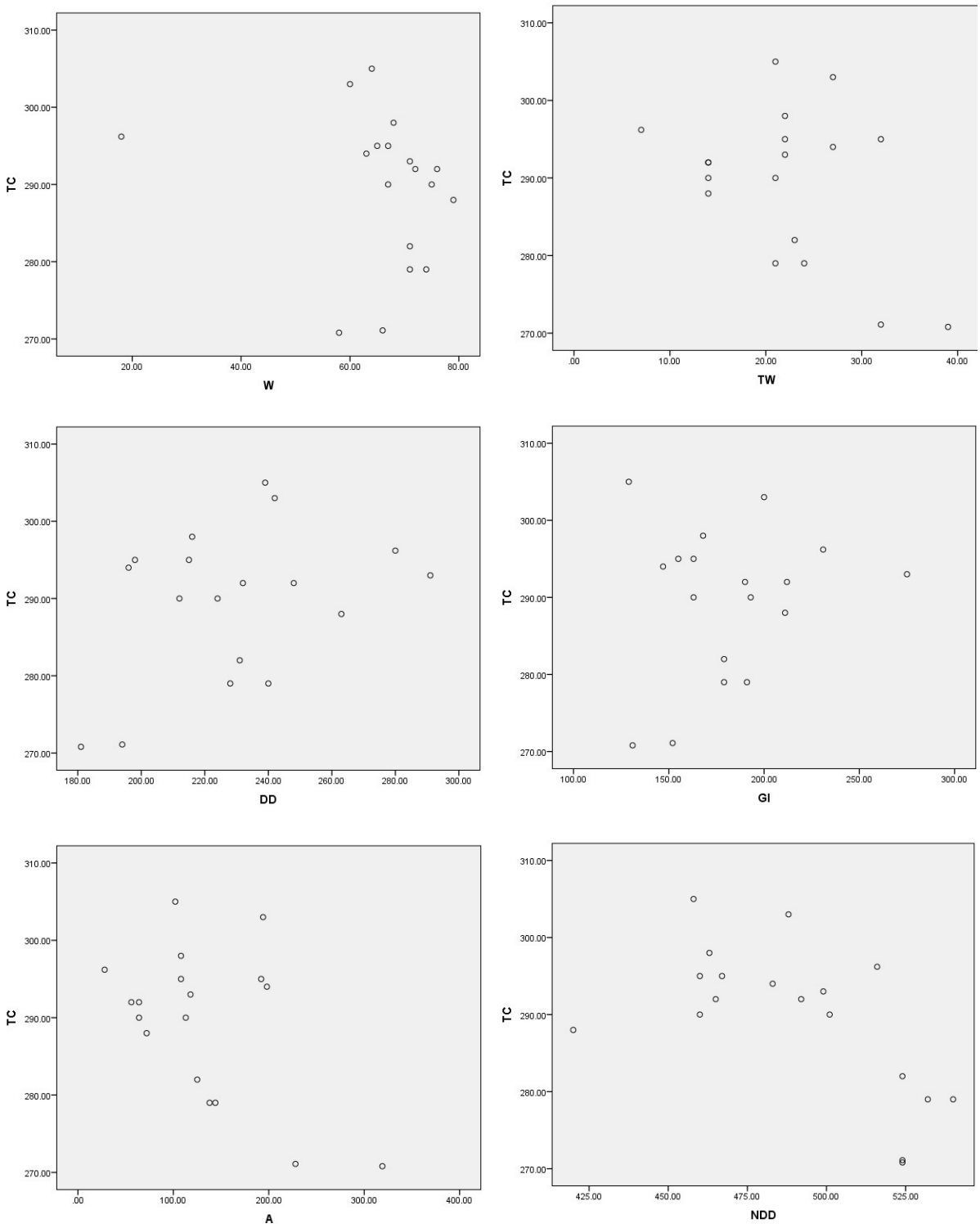
| Alkane | AF | DHVAP | BP | TC | PC | S | D | $R_m^2$ | $-\Delta H_f$ | $-\Delta H_v$ |
|---|---|---|---|---|---|---|---|---|---|---|
| n-octane | 0.3978 | 9.915 | 125.70 | 296.20 | 24.64 | 111.67 | 0.7025 | 2.0449 | 208.6 | 41.49 |
| 2M | 0.3779 | 9.484 | 117.6 | 288.0 | 24.80 | 109.84 | 0.6980 | 1.8913 | 215.4 | 39.67 |
| 3M | 0.3710 | 9.521 | 118.9 | 292.0 | 25.60 | 111.26 | 0.7058 | 1.7984 | 212.5 | 39.83 |
| 4M | 0.3715 | 9.483 | 117.7 | 290.0 | 25.60 | 109.32 | 0.7046 | 1.7673 | 210.7 | 39.64 |
| 3E | 0.3624 | 9.476 | 118.5 | 292.0 | 25.74 | 109.43 | 0.7136 | 1.7673 | 210.7 | 39.64 |
| 22MM | 0.3394 | 8.915 | 106.8 | 279.0 | 25.60 | 103.42 | 0.6953 | 1.6744 | 224.6 | 37.28 |
| 23MM | 0.3482 | 9.272 | 115.6 | 293.0 | 26.60 | 108.02 | 0.7121 | 1.6464 | 213.8 | 38.78 |
| 24MM | 0.3442 | 9.029 | 109.4 | 282.0 | 25.80 | 106.98 | 0.7004 | 1.6142 | 219.2 | 37.76 |
| 25MM | 0.3568 | 9.051 | 109.1 | 279.0 | 25.00 | 105.72 | 0.6935 | 1.6449 | 222.5 | 37.85 |
| 33MM | 0.3225 | 8.973 | 112.0 | 290.8 | 27.20 | 104.74 | 0.7100 | 1.7377 | 220.0 | 37.53 |
| 34MM | 0.3403 | 9.316 | 117.7 | 298.0 | 27.40 | 106.59 | 0.7200 | 1.5230 | 212.8 | 38.97 |
| 2M3E | 0.3324 | 9.209 | 115.6 | 295.0 | 27.40 | 106.06 | 0.7193 | 1.5525 | 211.0 | 38.52 |
| 3M3E | 0.3068 | 9.081 | 118.3 | 305.0 | 28.90 | 101.48 | 0.7274 | 1.5212 | 214.8 | 37.99 |
| 223MMM | 0.3008 | 8.826 | 109.8 | 294.0 | 28.20 | 101.31 | 0.7161 | 1.4306 | 220.0 | 36.91 |
| 224MMM | 0.3053 | 8.402 | 99.24 | 271.1 | 25.50 | 104.09 | 0.6919 | 1.4010 | 224.0 | 35.14 |
| 233MM | 0.2931 | 8.897 | 114.8 | 303.0 | 29.00 | 102.06 | 0.7262 | 1.4931 | 216.3 | 37.27 |
| 234MMM | 0.3174 | 9.014 | 113.5 | 295.0 | 27.60 | 102.39 | 0.7191 | 1.3698 | 217.3 | 37.75 |
| 2233MMMM | 0.2552 | 8.41 | 106.5 | 270.8 | 24.50 | 93.06 | 0.8242 | 1.4612 | 225.6 | 42.90 |

The values of $W$, $TW$, $DD$, $GI$, $\mathcal{A}$, $NDD$ and $NGI$ for the set of octane isomers are given in Table 2.

**Table 2**- Values of $NDD$ and $NGI$ for the set of octane isomers.

| S.No. | Alkane | $W(G)$ | $TW(G)$ | $DD(G)$ | $GI(G)$ | $\mathcal{A}(G)$ | $NDD(G)$ | $NGI(G)$ |
|---|---|---|---|---|---|---|---|---|
| 1 | n-octane | 18.00 | 7.00 | 280.00 | 231.00 | 28.00 | 516.00 | 781.00 |
| 2 | 2M | 79.00 | 14.00 | 263.00 | 211.00 | 72.00 | 420.00 | 663.00 |
| 3 | 3M | 76.00 | 14.00 | 248.00 | 212.00 | 64.00 | 492.00 | 785.00 |
| 4 | 4M | 75.00 | 14.00 | 224.00 | 193.00 | 64.00 | 460.00 | 751.00 |
| 5 | 3E | 72.00 | 14.00 | 232.00 | 190.00 | 56.00 | 465.00 | 779.00 |
| 6 | 22MM | 71.00 | 21.00 | 228.00 | 179.00 | 138.00 | 532.00 | 993.00 |
| 7 | 23MM | 71.00 | 22.00 | 291.00 | 275.00 | 118.00 | 499.00 | 839.00 |
| 8 | 24MM | 71.00 | 23.00 | 231.00 | 179.00 | 125.00 | 524.00 | 867.00 |
| 9 | 25MM | 74.00 | 24.00 | 240.00 | 191.00 | 144.00 | 540.00 | 968.00 |
| 10 | 33MM | 67.00 | 21.00 | 212.00 | 163.00 | 113.00 | 501.00 | 877.00 |
| 11 | 34MM | 68.00 | 22.00 | 216.00 | 168.00 | 108.00 | 463.00 | 664.00 |
| 12 | 2M3E | 67.00 | 22.00 | 215.00 | 163.00 | 108.00 | 460.00 | 771.00 |
| 13 | 3M3E | 64.00 | 21.00 | 239.00 | 129.00 | 102.00 | 458.00 | 825.00 |
| 14 | 223MMM | 63.00 | 27.00 | 196.00 | 147.00 | 198.00 | 483.00 | 936.00 |
| 15 | 224MMM | 66.00 | 32.00 | 194.00 | 152.00 | 228.00 | 524.00 | 970.00 |
| 16 | 233MM | 60.00 | 27.00 | 242.00 | 200.00 | 194.00 | 488.00 | 943.00 |
| 17 | 234MMM | 65.00 | 32.00 | 198.00 | 155.00 | 192.00 | 467.00 | 824.00 |
| 18 | 2233MMMM | 58.00 | 39.00 | 181.00 | 131.00 | 319.00 | 524.00 | 1177.00 |

In the following figure the correlation coefficient value for the critical temperature of octane isomers with the above mentioned topological indices are shown.


TC
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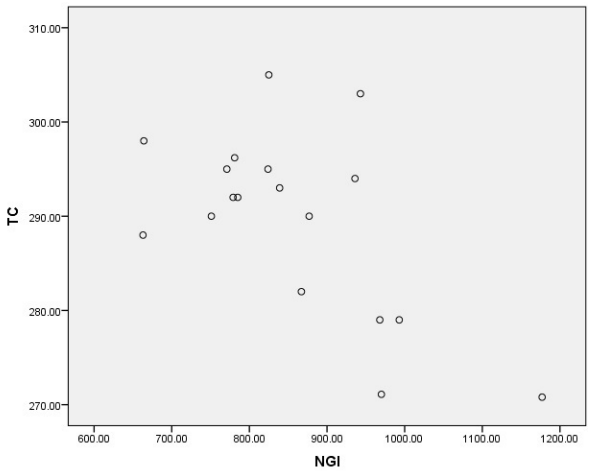


The neighborhood degree distance index and the neighborhood Gutman index shows good correlation with the set of octane isomers. Specially, for the critical temperature of the set of octane isomers, the correlation coefficient value of $NDD(G)$ and $NGI(G)$ are 0.610 and 0.605 respectively. Where as the correlation coefficient value of so called Wiener index is 0.189 which is almost five times less than the $NDD$ and $NGI$. Similarly, the correlation coefficient values for other parameters viz., $TW$, $DD$, $GI$ and $\mathcal{A}$ are 0.407, 0.307, 0.176 and 0.486 respectively. Clearly, we can see that the predicting power of $NDD$ and $NGI$ are far better than the already existing parameters.

## 3 $NDD$ and $NGI$ Indices of some graph operations

For a graph $G = (V, E)$, the Mycielskian of $G$ is the graph $\mu(G)$(or simply $\mu$) is defined as the graph having vertex set $V \cup X \cup \{x\}$ and edge set $E \cup \{v_i x_j : v_i v_j \in E\} \cup \{x_i x_j : 1 \leq j \leq n\}$, where $V = \{v_1, v_2, \cdots, v_n\}$ and $X = \{x_1, x_2, \cdots, x_n\}$.

For more details on Mycielskian graph see [1, 2]. In this paper we determine the exact value of the degree distance of Mycielskian graph with diameter. Also we determine exact value of degree distance of the complement of arbitrary Mycielskian graphs.

## 4 Results

We begin with the following straightforward, previously known, auxiliary result.

**Observation 1.** *Let $\mu$ be the Mycielskian of $G$. Then for each $v \in V(\mu)$ we have*

$$N_\mu(v) = \begin{cases} n + r(3r+1), & v = x; \\ n(r+1), & v = x_i; \\ 2r^2 + n, & v = v_i. \end{cases}$$

**Observation 2.** [2] *In the Mycielskian $\mu$ of $G$, the distance between two vertices $u, v \in V(\mu)$ are given as follows*

$$d_\mu(u,v) = \begin{cases} 1 & u = x, v = x_i \\ 2 & u = x, v = v_i \\ 2 & u = x_i, v = x_j \\ d_G(v_i, v_j) & u = v_i, v = v_j, d_G(v_i, v_j) \leq 3 \\ 4 & u = v_i, v = v_j, d_G(v_i, v_j) \geq 4 \\ 2 & u = v_i, v = x_j, i = j \\ d_G(v_i, v_j) & u = v_i, v = x_j, i \neq j, d_G(v_i, v_j) \leq 2 \\ 3 & u = v_i, v = x_j, i \neq j, d_G(v_i, v_j) \geq 3 \end{cases}$$

*Specially, the diameter of the Mycielskian graph is at most four.*

Now, we are in a position to establish the exact value of the degree distance of Mycielskian graph $\mu(G)$ of a graph $G$.

**Theorem 3.** *Let $G$ be a $(n,m)$-graph with $diam(G) = 2$. If $\mu$ is the Mycielskian of $G$, then the distance degree sum of $\mu$ is given by*

$$\begin{aligned} NDD(\mu) &= n[n(r+1) + 2r^2 + 1] + 2n[n(r+1) + n + r(3r+1)] + 4n[r^2+1] \\ &+ 2[n + r(3r+1)]W(G) + 2n[n + r(3r+1) + 2r^2 + n] + [n + r(3r+1) \\ &+ 2r^2 + n]\sum_{\{v_i, x_j\} \subseteq V(\mu)_{i \neq j}} d_\mu(v_i, x_j). \end{aligned}$$

*Proof.* We consider the following different possible cases.

**Case 1.** $u = x$ and $v \in X$.

$$\begin{aligned} \sum_{i=1}^{n} d_\mu(x, x_i)[deg_\mu(x) + deg_\mu(x_i)] &= \sum_{i=1}^{n} 1[n(r+1) + 2r^2 + 1] \\ &= n[n(r+1) + 2r^2 + 1]. \end{aligned}$$

**Case 2.** $u = x$ and $v \in V$.

$$\begin{aligned} \sum_{i=1}^{n} d_\mu(x, v_i)[deg_\mu(x) + deg_\mu(v_i)] &= \sum_{i=1}^{n} 2[n(r+1) + n + r(3r+1)] \\ &= 2n[n(r+1) + n + r(3r+1)]. \end{aligned}$$

**Case 3.** $\{u, v\} \subseteq X$.

Using Lemma 1, we have

$$\sum_{\{x_i, x_j\} \subseteq X} d_\mu(x_i, x_j)[deg_\mu(x_i) + deg_\mu(x_j)] = \sum_{\{x_i, x_j\} \subseteq X} 2[2r^2 + 1 + 2r^2 + 1]$$

$$= \quad 4[r^2+1].$$

**Case 4.** $\{u, v\} \subseteq V$.

$$\begin{aligned}\sum_{\{v_i,v_j\}\subseteq V} d_\mu(v_i,v_j)[deg_\mu(v_i)+deg_\mu(v_j)] &= \sum_{\{v_i,v_j\}\subseteq V} d_G(v_i,v_j)2[n+r(3r+1)] \\ &= 2[n+r(3r+1)]W(G).\end{aligned}$$

**Case 5.** $u = v_i$ and $v = x_i$, $1 \leq i \leq n$

$$\begin{aligned}\sum_{i=1}^{n} d_\mu(v_i,x_i)[deg_\mu(v_i)+deg_\mu(x_i)] &= \sum_{i=1}^{n} 2[n+r(3r+1)+2r^2+n] \\ &= 2n[n+r(3r+1)+2r^2+n].\end{aligned}$$

**Case 6.** $u = v_i$ and $v = x_j$, $i \neq j$

$$\begin{aligned}\sum_{\{v_i,x_j\}\subseteq V(\mu)_{i\neq j}} d_\mu(v_i,x_j)[deg_\mu(v_i)+deg_\mu(x_j)] &= \sum_{\{v_i,x_j\}\subseteq V(\mu)_{i\neq j}} d_\mu(v_i,x_j)[n+r(3r+1)+2r^2+n] \\ &= [n+r(3r+1)+2r^2+n]\sum_{\{v_i,x_j\}\subseteq V(\mu)_{i\neq j}} d_\mu(v_i,x_j).\end{aligned}$$

Hence

$$\sum_{\{v_i,x_j\}\subseteq V(\mu)_{i\neq j}} d_\mu(v_i,x_j)^2[deg_\mu(v_i)+deg_\mu(x_j)] = [n+r(3r+1)+2r^2+n]\sum_{\{v_i,x_j\}\subseteq V(\mu)_{i\neq j}} d_\mu(v_i,x_j).$$

Thus, the result follows by combining these cases. □

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