Generalized Second Neighborhood Zagreb Index: Mathematical Inequalities and Chemical Applicability of PAHs

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Abstract

Topological indices are graphical invariants that relate a numeric number to a graph, which is structurally invariant and predicts the chemical, biological and physical features of the molecular graphs. In this work, mathematical inequalities of generalized second neighborhood Zagreb index are obtained. Further, generalized second neighborhood Zagreb indices for some particular values are computed for some basic polycyclic aromatic hydrocarbons, and the QSPR analysis are also obtained.

Keywords: Chemical graph; Neighborhood Zagreb indices; Zagreb indices, Generalized second neighborhood Zagreb index; Regression Models

1. Introduction

In this paper we are concerned with simple graphs that is graphs without multiple, directed, or weighted edges, and without self-loops. Let $G(V, E)$ be such a graph with vertex set $V(G)$ and edge set $E(G)$. Let $|V(G)| = p$ and $|E(G)| = q$. The degree $d_G(v)$ of a vertex $v$ is the number of vertices adjacent to $v$. The set of all vertices which are adjacent to a vertex $v$ is called open neighborhood of $v$ and denoted by $N_G(v)$. The closed neighborhood set of a vertex $v$ is the set $N_G(v) = d_G(u) \cup \{v\}$. For graph-theoretical terminology and notation not defined here we follow [12].

Chemical graph theory is a branch of mathematical chemistry deals with the chemical graph obtained by considering molecules or atoms as vertices and chemical bonds as edge. Topological indices are numeric quantities that transform chemical structure to real number, which are used in QSAR/QSPR studies to correlate the bioactivity and physiochemical properties of molecule. For their history, applications and mathematical properties, see [2, 11, 14, 25, 26] and the references cited therein.

For any real number $\alpha$, the generalized second neighborhood Zagreb index $NZ_2^{(\alpha)}(G)$ is defined as $NZ_2^{(\alpha)}(G) = \sum_{u \in E(G)} [S_G(u)S_G(u)]^{\alpha}$, where $S_G(v) = \sum_{u \in N_G(v)} d_G(u)$ is the degree sum of neighbour vertices of $v$ in $V(G)$. This descriptor is defined by[17] and studied by [18-23].

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2. Mathematical Inequalities

In this section, we obtain some mathematical inequalities of $NZ_2^{(α)}(G)$ in terms of order, size, minimum/maximum degree, minimum/maximum neighborhood degree sum and generalized Randic index of a graph $G$. For more details, we refer [1, 3, 7, 8, 9, 15, 16].

Let $G$ be a non-trivial $(p, q)$ - graph with $α > 0$.

1. Since $1 \leq \{S_G(u), S_G(v)\} \leq (p - 1)^2$ for each $uv \in E(G)$, we have an inequality $NZ_2^{(α)}(G)$ in terms of order and size as

$$q \leq NZ_2^{(α)}(G) \leq q(p-1)^{4α},$$

2. Since $δ(G)^2 \leq \{S_G(u), S_G(v)\} \leq Δ(G)^2$ for each edge $uv \in E(G)$, we have an inequality $NZ_2^{(α)}(G)$ in terms of size and minimum/maximum degree of $G$ as

$$qδ(G)^4 \leq NZ_2^{(α)}(G) \leq qΔ(G)^4.$$

3. Since $δ_n(G) = \{S_G(u), S_G(v)\} \leq Δ_n(G)$ for all vertices $u, v \in V(G)$, where

$Δ_n(G) = \max\{S_G(v) : v \in V(G)\}$ and $δ_n(G) = \min\{S_G(v) : v \in V(G)\}$. Hence, we have an inequality $NZ_2^{(α)}(G)$ in terms of size and neighborhood degree sum as

$$qδ_n(G)^4 \leq NZ_2^{(α)}(G) \leq qΔ_n(G)^4.$$

4. Since $d_G(u) \leq S_G(u) \leq Δ(G)d_G(u)$ and $d_G(v) \leq S_G(v) \leq Δ(G)d_G(v)$ for each edge $uv \in E(G)$, we have an inequality $NZ_2^{(α)}(G)$ in terms of size, degree and $R_α(G)$ as

$$R_α(G) \leq NZ_2^{(α)}(G) \leq qΔ(G)^αR_α(G),$$

where the generalized Randic index of a graph $G$, see [10] is denoted and defined by

$R_α(G) = \sum_{uv \in E(G)}[d_G(u)d_G(v)]^α$.

5. The sum and product of $NZ_2^{(α)}(G)$ and $NZ_2^{(α)}(\tilde{G})$ of a connected graph $G$ and $\tilde{G}$ in terms of order, we have

(i) $p(p-1)/2 \leq NZ_2^{(α)}(G) + NZ_2^{(α)}(\tilde{G}) \leq p(p-1)^{4α+1}/2$,  
(ii) $p(p-1)/4 \leq NZ_2^{(α)}(G)NZ_2^{(α)}(\tilde{G}) \leq p^2(p-1)^{4α+2}/16$, 

where the complementary graph $\tilde{G}$ of a graph $G$ with vertex set $V(G)$ and $m \in E(\tilde{G})$ if and only if $m \in E(G)$. Note that, $q + \tilde{q} = p(p-1)/2$ and $(q + \tilde{q})/2 \leq q\tilde{q} \leq (q + \tilde{q})^2/4$, where $\tilde{q}$ is the number of edges of $\tilde{G}$.

3. Chemical Applicability

The properties and activities of chemicals are strongly related to their molecular structures, which are capable to predict the higher correlation factor has greater importance in quantitative structure-property relationships (QSPR).

3.1. Polycyclic Aromatic Hydrocarbons (PAHs)

Polycyclic aromatic hydrocarbons (PAHs) are the primary source of environmental pollution and most are carcinogenic and mutagenic. The accumulation and influence of PAHs on the environment and human health depends on their physico-chemical properties. Therefore, the QSPR study of physical and chemical properties helps to manage these PAHs. Recently the QSPR analysis of PAHs was studied in [5, 6]. In this paper, we examined the chemical graph of certain fundamental PAHs.

3.2. Theoretical Data set

The generalized second neighborhood Zagreb indices for $α \in \left\{1, 2, \frac{1}{2}, -\frac{1}{2}\right\}$ analogous to the second zagreb index $M_2(G)$, the second hyper zagreb index $HM_2(G)$, the reciprocal randic index $RR(G)$, the randic index $R(G)$ are studied in this article. Let $S_G(v) = \sum_{u \in N_G(v)} d_G(u)$ be the degree sum of neighbour vertices.
\( v \in V(G) \), and the neighborhood partition \( \text{NE}_{i,j} = \{uv \in E(G): S_G(u) = i \& S_G(v) = j \} \) and \( N(i,j) = |\text{NE}_{i,j}| \). The edge partition of PAHs is given in the Table-1.

### Table-1: Bond partition for molecular graphs of PAHs

| Sl No | Aromatic hydro carbons | Edge partition and their cardinality |
|-------|------------------------|-------------------------------------|
| 1     | Naphthalene (Nap)      | \((4, 4)\) \((5, 4)\) \((7, 5)\) \((7,7)\) \| 2 4 4 4 1 |
| 2     | Acenaphthylene (Ace)   | \((5, 4)\) \((5, 4)\) \((5, 5)\) \((9, 7)\) \| 4 6 1 3 |
| 3     | Fluorene (Fle)         | \((4, 4)\) \((5, 4)\) \((8, 5)\) \((7, 5)\) \((5, 5)\) \((7, 6)\) \((8,7)\) \| 2 4 2 3 1 2 1 |
| 4     | Phenanthrene (Phe)     | \((4, 4)\) \((5, 4)\) \((8, 5)\) \((8,6)\) \((6, 5)\) \((7, 5)\) \((5, 5)\) \((7, 6)\) \((8, 4)\) \| 2 6 1 1 1 1 2 1 1 |
| 5     | Fluoranthenne (Flu)    | \((4, 4)\) \((5, 4)\) \((8, 5)\) \((8,8)\) \((7, 5)\) \((9, 8)\) \((9, 7)\) \| 1 6 4 3 2 2 1 |
| 6     | Pyrene (Pyr)           | \((5, 4)\) \((7, 5)\) \((5, 5)\) \((9, 7)\) \((9, 9)\) \| 4 8 2 4 1 |
| 7     | Anthracene (Ant)       | \((4, 4)\) \((5, 4)\) \((7, 5)\) \((7,6)\) \((7, 5)\) \((7,7)\) \| 2 4 2 2 4 2 2 |
| 8     | Benzo(a)anthracene     | \((4, 4)\) \((5, 4)\) \((8, 5)\) \((8,8)\) \((8,6)\) \((7, 5)\) \((7, 6)\) \((5, 5)\) \((8,7)\) \((7,7)\) \| 2 4 1 1 5 3 1 2 1 |
| 9     | Chrysene (Chr)         | \((4, 4)\) \((5, 4)\) \((7, 5)\) \((5, 5)\) \((8, 5)\) \((8, 8)\) \((8,7)\) \| 2 4 4 2 4 3 2 |
| 10    | Benzo(b)fluoranthene   | \((4, 4)\) \((5, 4)\) \((7, 5)\) \((7,6)\) \((8,6)\) \((8,8)\) \((8,5)\) \((8,7)\) \((9, 8)\) \| 2 6 1 1 1 4 5 1 3 |
| 11    | Benzo(k)fluoranthene   | \((5, 4)\) \((7, 5)\) \((8, 5)\) \((8,8)\) \((8,6)\) \((7, 6)\) \((4, 4)\) \((9, 7)\) \((9, 8)\) \((7,7)\) \| 6 4 2 3 2 2 1 1 2 1 |
| 12    | Benzo(a)pyrene         | \((5, 4)\) \((7, 5)\) \((5, 5)\) \((7,6)\) \((4, 4)\) \((8, 5)\) \((8, 8)\) \((8,9)\) \((9, 9)\) \((8,7)\) \| 5 6 2 2 1 2 1 1 3 1 |
| 13    | Dibenzo(a,h)anthracene | \((5, 4)\) \((7, 5)\) \((5, 5)\) \((7,6)\) \((8,6)\) \((8,8)\) \((8,5)\) \((8,7)\) \((4, 4)\) \((8,7)\) \| 4 6 2 2 2 2 2 2 4 1 |
| 14    | Benzo(g,h,i)perylyne   | \((5, 4)\) \((7, 5)\) \((5, 5)\) \((8, 5)\) \((8,8)\) \((8,9)\) \((9, 9)\) \((9, 9)\) \((9, 7)\) \| 5 8 3 2 1 2 3 3 4 |
| 15    | Indeno(1,2,3-cd)pyrene | \((5, 4)\) \((7, 5)\) \((8, 5)\) \((8,7)\) \((4, 4)\) \((8, 8)\) \((8,5)\) \((9, 7)\) \((9, 9)\) \| 4 7 3 1 1 1 2 4 2 2 |

The generalized second neighbor index of Naphthalene for \( \alpha = 1 \) is calculated as follows:

\[
NZ_2^{(\alpha)}(G) = \sum_{uv \in E(G)} [S_G(u)S_G(v)]^\alpha = 2(4 \cdot 4) + 4(5 \cdot 4) + 4(7 \cdot 5) + 1(7 \cdot 7) = 301.
\]

Similarly, we have Table-2.
Table-2 \(NZ_2^{(\alpha)}\) for molecular graphs of PAHs

3.3. Experimental Data set

The physical and chemical properties, Water solubility(\(WF_3\)) in \(mg/l\), Octane water partitioning co-efficient(\(OW\)), Organic carbon-water partitioning co-efficient(\(OC\)), Henry constant(\(HC\)) in \(PaM^3/mol\), Boiling Point(\(BP\)) in \(^\circ\)C, Melting point(\(MP\)) in \(^\circ\)C, Density(\(D\)) in \(g/cm^3\), Enthalpy of vaporization (\(EV\)) in \(kJ/mol\), Flash point(\(FP\)) in \(^\circ\)C, Index of Refraction(\(IR\)), Molar Refractivity(\(MR\)) in \(cm^3\), Polarization(\(P\)) in \(cm^3\), Surface tension(\(ST\)) in dyne/cm, Molar Value(\(MV\)) in \(cm^3\) are taken from \([4,13,24]\) and tabulated in the Table-3.

| PAHs | WS | OW | OC | HC | BP | MP | D | EV | FP | IR | MR | P | ST | MV |
|------|----|----|----|----|----|----|---|----|----|----|----|---|----|----|
| Nap  | 31.7 | 3.4 | 3.1 | 48.9 | 218 | 80 | 1 | 43.9 | 78.9 | 1.63 | 44.1 | 17.5 | 40.2 | 123.5 |
| Ace  | 3.93 | 4 | 1.4 | 15.7 | 280 | 89.4 | 1.2 | 51.7 | 137.2 | 1.73 | 51.3 | 20.3 | 54.7 | 128.2 |
| Fle  | 1.83 | 4.5 | 3.9 | 7.75 | 294 | 114.76 | 1.1 | 51.2 | 133.1 | 1.65 | 53.8 | 21.3 | 46.2 | 148.3 |
| Phe  | 1.2 | 4.5 | 4.2 | 3.981 | 338.4 | 99 | 1.1 | 55.8 | 146.6 | 1.72 | 61.9 | 24.6 | 48 | 157.7 |
| Flu  | 0.23 | 5.2 | 4.6 | 0.659 | 384 | 230 | 1.2 | 59.8 | 168.4 | 1.85 | 72.5 | 28.7 | 59.4 | 162 |
| Pyr  | 0.0013 | 5.2 | 4.6 | 1.1 | 404 | 151 | 1.2 | 63 | 168.8 | 1.85 | 72.5 | 28.7 | 59.4 | 162 |
| Ant  | 0.076 | 4.5 | 4.2 | 7.19 | 342 | 218 | 1.1 | 55.8 | 146.6 | 1.72 | 61.9 | 24.6 | 48 | 157.7 |
| BaA  | 0.01 | 5.9 | 5.3 | 0.248 | 437.6 | 156 | 1.2 | 67.9 | 209.1 | 1.77 | 79.8 | 31.6 | 33.5 | 191.8 |
| Chr  | 0.0028 | 5.9 | 5.3 | 0.1064 | 448 | 255 | 1.2 | 67.9 | 209.1 | 1.77 | 79.8 | 31.6 | 33.5 | 191.8 |
| BbF  | 0.012 | 6.6 | 6.7 | 1.236 | 481 | 168 | 1.3 | 70.2 | 228.6 | 1.89 | 90.3 | 35.8 | 63.5 | 196.1 |
| BkF  | 7.60E-04 | 6.1 | 5.7 | 0.111 | 480 | 217 | 1.3 | 71.6 | 228.6 | 1.89 | 90.3 | 35.8 | 63.5 | 196.1 |
| BaP  | 0.0023 | 6.5 | 6.7 | 0.5 | 496 | 178.1 | 1.3 | 73.4 | 228.6 | 1.89 | 90.3 | 35.8 | 63.5 | 196.1 |
| DBA  | 0.0025 | 6.5 | 6.5 | 0.0074 | 524 | 267 | 1.2 | 76.9 | 264.5 | 1.81 | 97.6 | 38.7 | 57.7 | 225.9 |
| BghiPe | 0.062 | 7.1 | 6.2 | 0.0146 | 550 | 278 | 1.4 | 74.1 | 247.2 | 2.01 | 100.8 | 40 | 74.2 | 200.4 |
| IDP  | 2.60E-07 | 6.6 | 6.2 | 0.162 | 536 | 164 | 1.5 | 86.8 | 264.8 | 2.05 | 102.7 | 40.7 | 84.7 | 198.8 |

Table - 3: PAHs with their Physico-chemical properties
3.4. Linear and non-linear regression model for PAHs

We have tested the linear and non-linear regression models for the values of fourteen Physico-chemical properties and $NZ_2^{(a)}$ for $a \in \{1, 2, \frac{1}{2}, -\frac{1}{2}\}$ of fifteen PAHs using SSPS software. The study of the Table - 4 reveals that the index $NZ_2^{(1)}$ has good correlation with all properties except $WS$, $MP$ and $ST$ in both linear and non-linear models. $MR$ and $P$ have the highest value of $R$ as 0.975 and 0.976 in linear and non-linear regression models respectively. The figures in the table - 5 shows the chemical properties strongly correlated with $NZ_2^{(1)}$ for $R$ greater than 0.9.

| Properties | Linear | Non-linear |
|------------|--------|------------|
|            | $R$    | Rsquare    | $F$ | $P$ | $R$    | Rsquare    | $F$ | $P$ |
| WS         | .533   | .284       | 5.166 | .041 | .773   | .598       | 8.908 | .004 |
| OW         | .957   | .916       | 142.004 | .000 | .964   | .930       | 79.466 | .000 |
| OC         | .825   | .680       | 27.663 | .000 | .829   | .688       | 13.235 | .001 |
| HC         | .651   | .423       | 9.544 | .009 | .845   | .714       | 14.954 | .001 |
| BP         | .963   | .928       | 166.958 | .000 | .969   | .940       | 93.589 | .000 |
| MP         | .658   | .433       | 9.937 | .008 | .709   | .503       | 6.078  | .015 |
| D          | .921   | .848       | 72.506 | .000 | .930   | .865       | 38.392 | .000 |
| EV         | .949   | .901       | 118.731 | .000 | .950   | .903       | 55.627 | .000 |
| FP         | .950   | .903       | 121.155 | .000 | .958   | .917       | 66.572 | .000 |
| IR         | .937   | .878       | 93.824 | .000 | .873   | .043       | 49.038 | .000 |
| MR         | .975   | .951       | 252.670 | .000 | .976   | .953       | 121.918 | .000 |
| P          | .975   | .950       | 248.043 | .000 | .976   | .952       | 119.076 | .000 |
| ST         | .533   | .284       | 5.162 | .041 | .773   | .598       | 8.908  | .004 |
| MV         | .866   | .750       | 39.003 | .000 | .886   | .786       | 21.979 | .000 |

Table - 4: Statistical parameters of linear and non-linear regression analysis for $NZ_2^{(1)}$

From the Table-6, the index $NZ_2^{(2)}$ has good correlation with all the properties other than $WS$, $OC$, $HC$ and $MP$ in both linear and non-linear models. It has the highest value of $R$ as 0.965 and 0.968 in linear and non-linear models respectively. The figures in the table - 7 shows the chemical properties strongly correlated with $NZ_2^{(2)}$ for $R$ greater than 0.9.
| Properties | Linear | | | Non-linear | | |
|------------|--------|--------|--------|------------|--------|--------|
|            | R      | Rsquare| F   | P  | R     | Rsquare| F   | P  |
| WS         | .480   | .231   | 3.901 | .070 | .668  | .447   | 4.845 | .029 |
| OW         | .916   | .838   | 67.381 | .000 | .931  | .866   | 38.790 | .000 |
| OC         | .760   | .578   | 17.823 | .001 | .773  | .598   | 8.916  | .004 |
| HC         | .593   | .352   | 7.055  | .020 | .753  | .567   | 7.862  | .007 |
| BP         | .917   | .841   | 68.811 | .000 | .932  | .868   | 39.357 | .000 |
| MP         | .613   | .376   | 7.832  | .015 | .683  | .466   | 5.246  | .023 |
| D          | .942   | .888   | 103.021 | .000 | .947  | .898   | 52.668 | .000 |
| EV         | .906   | .822   | 59.903  | .000 | .912  | .832   | 29.721 | .000 |
| FP         | .895   | .801   | 52.459  | .000 | .914  | .836   | 30.594 | .000 |
| IR         | .965   | .931   | 175.791 | .000 | .968  | .937   | 88.717 | .000 |
| MR         | .935   | .875   | 90.738  | .000 | .942  | .887   | 47.110 | .000 |
| P          | .935   | .875   | 89.929  | .000 | .941  | .885   | 46.400 | .000 |
| ST         | .942   | .888   | 103.275 | .000 | .953  | .908   | 58.976 | .000 |
| MV         | .784   | .615   | 20.768  | .001 | .825  | .681   | 12.796 | .001 |

**Table - 6:** Statistical parameters of linear and non-linear regression analysis for $NZ_2^{(2)}$

From the Table -8, $NZ_2^{(2)}$ is in good correlation with all the properties except $WS$, $HC$ and $MP$ in linear and except $MP$ in non-linear models. $MR$ and $P$ are having highest value of $R$ =0.990 in both the models. The figures in the table -9 shows the chemical properties strongly correlated with $NZ_2^{(1/2)}$ for R greater than 0.9.
Table - 8: Statistical parameters of linear and non-linear regression analysis for $NZ_2^{1/2}$

| Properties | Linear | Non-linear |
|------------|--------|------------|
|            | R      | Rsquare    | F    | P    | R      | Rsquare    | F    | P    |
| IR         | .912   | .832       | 64.359 | .000 | .919   | .844       | 32.394 | .000 |
| MR         | .990   | .981       | 659.043 | .000 | .990   | .981       | 310.132 | .000 |
| P          | .990   | .980       | 637.621 | .000 | .990   | .980       | 298.737 | .000 |
| ST         | .884   | .781       | 46.304  | .000 | .900   | .811       | 25.666  | .000 |
| MV         | .907   | .822       | 60.214  | .000 | .919   | .845       | 32.689  | .000 |

Table - 9: Physico-chemical properties best correlated with $NZ_2^{(-1/2)}$

The study of the table - 10 reveals that the index $NZ_2^{(-1/2)}$ has good correlation with all the properties except $WS$, $HC$, $MP$, $D$ and $ST$ in linear and except $MP$ and $ST$ in non-linear models. This index has the highest value of $R = 0.989$ for $BP$ in both linear and non-linear regression. The figures in the table - 11 shows the chemical properties strongly correlated with $NZ_2^{(-1/2)}$ for $R$ greater than 0.9.

| Properties | Linear | Non-linear |
|------------|--------|------------|
|            | R      | Rsquare    | F    | P    | R      | Rsquare    | F    | P    |
| WS         | .587   | .345       | 6.845 | .021 | .845   | .715       | 15.032 | .001 |
| OW         | .979   | .959       | 307.260 | .000 | .980   | .961       | 146.120 | .000 |
| OC         | .929   | .864       | 82.315 | .000 | .932   | .869       | 39.879  | .000 |
| HC         | .719   | .517       | 13.914 | .003 | .931   | .867       | 39.280  | .000 |
| BP         | .989   | .978       | 564.888 | .000 | .989   | .978       | 268.111 | .000 |
| MP         | .690   | .476       | 11.787 | .004 | .697   | .486       | 5.678   | .018 |
| D          | .798   | .637       | 22.850 | .000 | .805   | .649       | 11.083  | .002 |
| EV         | .959   | .919       | 148.055 | .000 | .960   | .921       | 69.822  | .000 |
| FP         | .983   | .966       | 366.425 | .000 | .983   | .966       | 170.593 | .000 |
| IR         | .811   | .659       | 25.069 | .000 | .815   | .664       | 11.868  | .001 |
| MR         | .988   | .977       | 544.279 | .000 | .989   | .978       | 266.917 | .000 |
| P          | .988   | .977       | 553.741 | .000 | .989   | .978       | 272.811 | .000 |
| ST         | .772   | .596       | 19.204 | .001 | .784   | .615       | 9.589   | .003 |
| MV         | .973   | .947       | 230.667 | .000 | .974   | .948       | 110.502 | .000 |

Table - 10: Statistical parameters of linear and non-linear regression analysis for $NZ_2^{(-1/2)}$
Table - 11: Physico-chemical properties best correlated with $NZ_2^{(-\frac{1}{2})}$.

4. Conclusion
In this article, some mathematical inequalities for generalized second neighborhood indices are obtained. We computed generalized second neighborhood Zagreb indices for $a = \{1, 2, 1/2, -1/2\}$ for PAHs and the QSPR analysis is performed for the Physico-chemical properties of the PAHs. It was found, the correlation between these indices with different properties of PAHs are often strong and hence these indices are suitable for QSPR analysis.

Conflict of Interest: The authors declare that there is no conflict of interest regarding the publication of this article.

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