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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*

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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 α, the generalized second neighborhood Zagreb index $NZ_2^{(\alpha)}(G)$ is defined as $NZ_2^{(\alpha)}(G) = \sum_{uv\in E(G)}[S_G(u)S_G(u)]^{\alpha}$, 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].

2. Mathematical Inequalities

In this section, we obtain some mathematical inequalities of $NZ_2^{(\alpha)}(G)$ 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 $\alpha > 0$.

1. Since $1 \leq \{S_G(u),\ S_G(v)\} \leq (p-1)^2$ for each $uv \in E(G)$, we have an inequality $NZ_2^{(\alpha)}(G)$ in terms of order and size as
$$q \leq NZ_2^{(\alpha)}(G) \leq q(p-1)^{4\alpha}.$$
2. Since $\delta(G)^2 \leq \{S_G(u),\ S_G(v)\} \leq \Delta(G)^2$ for each edge $uv \in E(G)$, we have an inequality $NZ_2^{(\alpha)}(G)$ in terms of size and minimum/maximum degree of *G* as
$$q\delta(G)^4 \leq NZ_2^{(\alpha)}(G) \leq q\Delta(G)^4.$$
3. Since $\delta_N(G) \leq \{S_G(u),\ S_G(v)\} \leq \Delta_N(G)$ for all vertices $u, v \in V(G)$, where $\Delta_N(G) = max\{S_G(v): v \in V(G)\}$ and $\delta_N(G) = min\{S_G(v): v \in V(G)\}$. Hence, we have an inequality $NZ_2^{(\alpha)}(G)$in terms of size and neighborhood degree sum as
$$q\delta_N(G)^4 \leq NZ_2^{(\alpha)}(G) \leq q\Delta_N(G)^4.$$
4. Since $d_G(u) \leq S_G(u) \leq \Delta(G)d_G(u)$ and $d_G(v) \leq S_G(v) \leq \Delta(G)d_G(v)$ for each edge $uv \in E(G)$, we have an inequality $NZ_2^{(\alpha)}(G)$ in terms of size, degree and $R_\alpha(G)$as
$$R_\alpha(G) \leq NZ_2^{(\alpha)}(G) \leq q\Delta(G)^\alpha R_\alpha(G),$$
where the generalized Randic index of a graph *G*, see [10] is denoted and defined by
$$R_\alpha(G) = \sum_{uv\in E(G)}[d_G(u)d_G(v)]^\alpha.$$
5. The sum and product of $NZ_2^{(\alpha)}(G)$ and $NZ_2^{(\alpha)}(\bar{G})$ of a connected graph *G* and $\bar{G}$ in terms of order , we have

(i) $\frac{p(p-1)}{2} \leq NZ_2^{(\alpha)}(G) + NZ_2^{(\alpha)}(\bar{G}) \leq \frac{p(p-1)^{4\alpha+1}}{2}$

(ii) $\frac{p(p-1)}{4} \leq NZ_2^{(\alpha)}(G)NZ_2^{(\alpha)}(\bar{G}) \leq \frac{p^2(p-1)^{4\alpha+2}}{16}$,

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

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 $\alpha \in \left\{1, 2, \frac{1}{2}, -\frac{1}{2}\right\}$ analogous to the 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 $NE_{i,j} = \{uv \in E(G): S_G(u) = i \,\&S_G(v) = j\}$ and $N(i,j) = |NE_{i,j}|$. The edge partition of PAHs is given in the Table-1.

Sl No.	Aromatic hydro carbons	Edge partition and their cardinality									
1	Napthalene (Nap)	(4, 4)	(5, 4)	(7, 5)	(7,7)						
		2	4	4	1						
2	Acenaphthelene (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	2	1	1	1	
5	Fluoranthene (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	4	2	2				
8	Benzo(a)anthracene (BaA)	(4, 4)	(5, 4)	(8, 5)	(8, 8)	(8,6)	(7, 5)	(7,6)	(5, 5)	(8,7)	(7,7)
		2	4	1	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 (BbF)	(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 (BkF)	(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 (BaP)	(5, 4)	(7, 5)	(5, 5)	(7,6)	(4, 4)	(8, 5)	(8, 8)	(9, 9)	(9, 7)	(8,7)
		5	6	2	2	1	2	1	1	3	1
13	Dibenzo(a,h)anthracene (DBA)	(5, 4)	(7, 5)	(5, 5)	(7,6)	(8,6)	(8, 8)	(8, 5)	(4, 4)	(8,7)	
		4	6	2	2	2	2	2	2	4	
14	Benzo(g,h,i)perylyne (BghiPe)	(5, 4)	(7, 5)	(5, 5)	(8, 5)	(8, 8)	(9, 8)	(9, 9)	(9, 7)		
		5	8	3	2	1	2	3	3		
15	Indeno(1,2,3-cd)pyrene (IDP)	(5, 4)	(7, 5)	(8, 5)	(8,7)	(4, 4)	(8, 8)	(5, 5)	(9, 7)	(9, 9)	(9, 8)
		4	7	3	1	1	1	2	4	2	2

Table-1: Bond partition for molecular graphs of PAHs

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

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

Similarly, we have Table-2.

PAHs	Particular values for $NZ_2^{(\alpha)}$			
	$NZ_2^{(1)}$	$NZ_2^{(2)}$	$NZ_2^{(1/2)}$	$NZ_2^{(-1/2)}$
Nap	301	9413	56.55286295	2.213407738
Ace	504	21482	82.19678432	2.48657677
Fle	462	16276	81.73068998	2.859984831
Phe	439	13579	82.53255437	3.19580817
Flu	765	38131	116.8710133	3.298848438
Pyr	743	35087	115.9661978	3.26173774
Ant	518	18870	89.47582575	2.97347828
BaA	751	30827	123.1305529	3.740061331
Chr	766	33222	123.8177138	3.745267369
BbF	1005	51277	150.7197749	4.087065981
BkF	984	47918	149.87195	4.060821352
BaP	930	43284	145.7628271	4.154759765
DBA	984	42784	156.7852801	4.506644381
BghiPe	1175	62929	173.1207532	4.458508629
IDP	1189	63079	174.4776615	4.422492531

Table-2 :$NZ_2^{(\alpha)}$ for molecular graphs of PAHs

3.3. Experimental Data set

The physical and chemical properties, Water solubility(*WS*) 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 $°C$, Melting point(*MP*) in$°C$, Density(*D*) in *g*/*cm*³, Enthalpy of vaporization (EV) in *kJ*$/mol$, Flash point(*FP*) in $°C$, Index of Refraction(*IR*), Molar Refractivity(*MR*) in *cm*³, Polarization(*P*) in *cm*³, Surface tension(*ST*) in *dyne*/*cm*³, 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	66.7	209.1	1.77	79.8	31.6	53.5	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	53.5	191.8
BbF	0.012	6.6	5.7	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 $NZ_2^{(\alpha)}$ for $\alpha\epsilon\left\{1,2,\frac{1}{2},-\frac{1}{2}\right\}$ 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	38.592	.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	5.166	.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 $NZ_2^{(1)}$

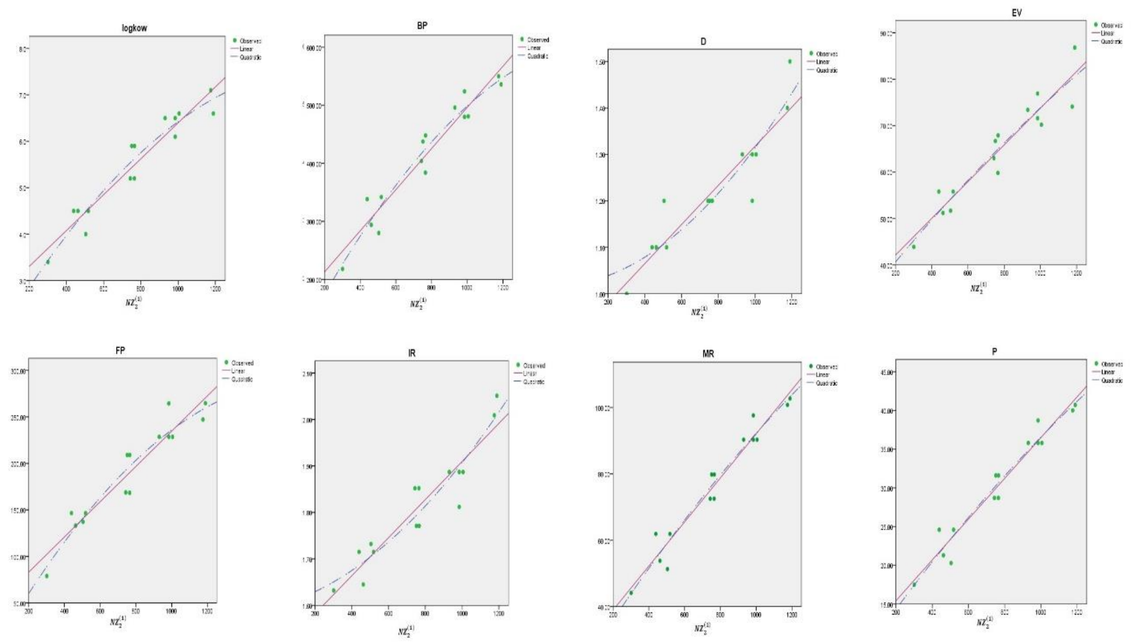

Table - 5: Physico-chemical properties best correlated with $NZ_2^{(1)}$

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	.874	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 $NZ_2^{(2)}$

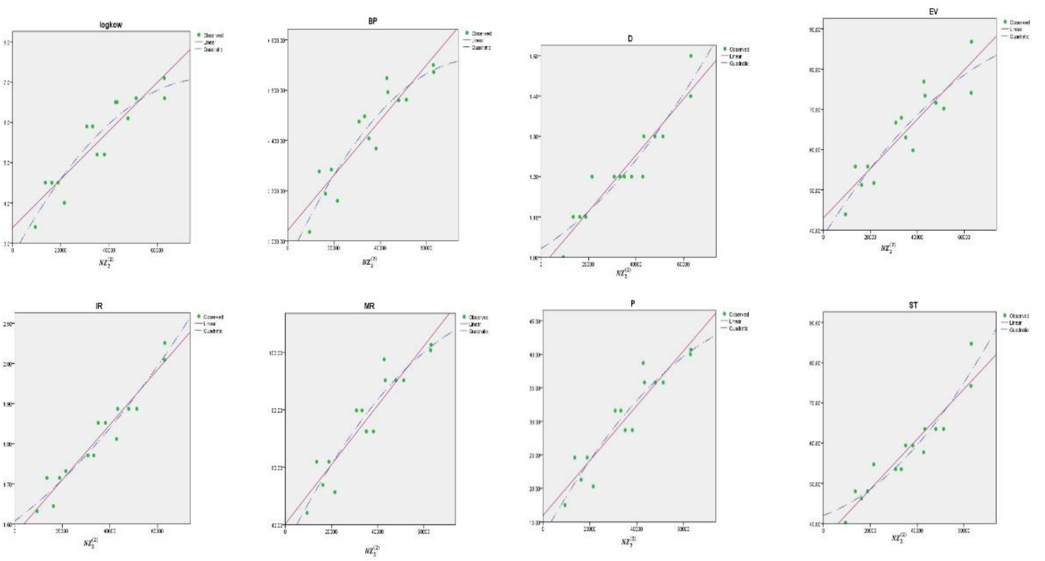

Table - 7: Physico-chemical properties best correlated with $NZ_2^{(2)}$

From the Table -8, $NZ_2^{(\frac{1}{2})}$ 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.

Properties	Linear				Non-linear			
	R	Rsquare	F	P	R	Rsquare	F	P
WS	.558	.312	5.892	.030	.830	.690	13.334	.001
OW	.974	.949	239.881	.000	.979	.958	136.313	.000
OC	.860	.740	36.983	.000	.863	.745	17.549	.000
HC	.679	.461	11.133	.005	.898	.807	25.008	.000
BP	.982	.965	357.443	.000	.986	.973	212.454	.000
MP	.677	.458	10.996	.006	.714	.509	6.222	.014
D	.898	.807	54.243	.000	.907	.823	27.872	.000
EV	.965	.931	176.298	.000	.965	.931	81.569	.000
FP	.973	.946	228.866	.000	.977	.954	123.233	.000

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 - 8: Statistical parameters of linear and non-linear regression analysis for $NZ_2^{(1/2)}$

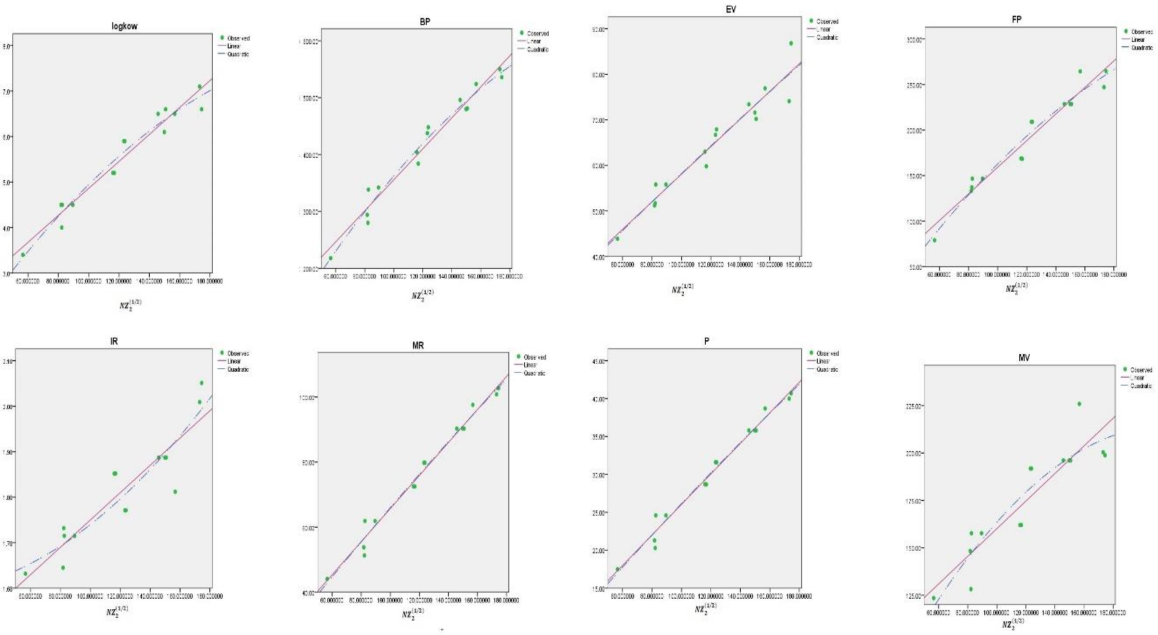

Table- 9: Physico-chemical properties best correlated with $NZ_2^{(-\frac{1}{2})}$

The study of the table - 10 reveals that the index $NZ_2^{(-\frac{1}{2})}$ 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 $NZ_2^{(-\frac{1}{2})}$ 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 $NZ_2^{(-1/2)}$

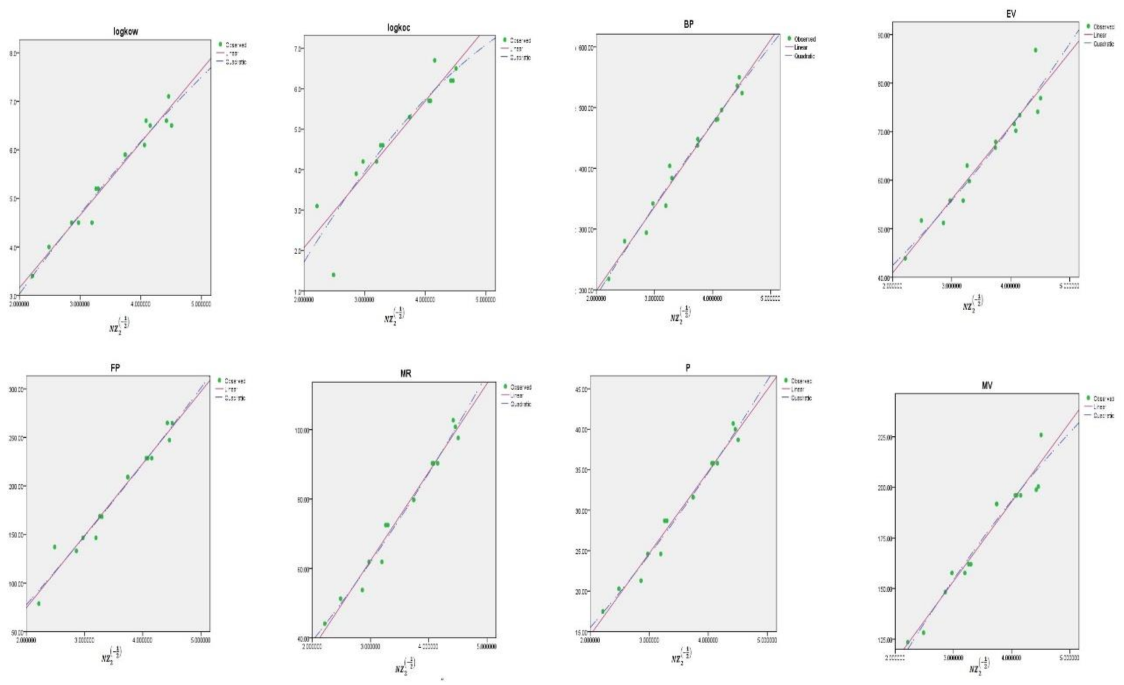

Table - 11: Physico-chemical properties best correlated with $NZ_2^{(-\frac{1}{2})}$.

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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