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The Pivotal Role of Degree-Based and Neighborhood Degree-Sum-Based Topological Indices in Predicting the Physico-Chemical Properties of N-Octane Isomers

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ABSTRACT

Neighborhood degree-sum topological index is sum of the degree of neighborhood vertices of the vertex u and is denoted as S_u where degree-based topological index is the number of edges meet at u and is denoted as d_u. In this paper, we have done the comparative analysis between ten notable degree-based indices with their corresponding neighborhood degree-sum topological indices. We report here, the correlation of mentioned types of topological indices with five Physico-chemical properties of octane isomers. Furthermore, we have discussed a deeper-lying relation between Augmented Zagreb Index with Atom-bond Connectivity Index based on the correlation with one of the Physico-chemical properties (boiling point) of octane isomers.

Keywords*:* Neighborhood degree-sum topological indices, degree of vertex, Physico-Chemical properties.

Introduction

Graph theory is the main branch of discrete mathematics which involves many applications to modeling real- life problems. Chemical graph theory has an important role in QSPR analysis through topological indices. Topological indices are the numbers associated with molecular graphs where atoms denote vertices and their respective chemical bonds denote edges. Degree-based topological index is the main branch of topological indices. It includes neighborhood degree-sum topological indices whose applications have been widespread in recent years. Eighteen octane structural isomers have been used in the study of QSPR/QSAR due to their structural discrimination and the availability of experimental values (Physico-Chemical properties). In 1975, Milan Randic set forth the first degree-based topological index in his seminal paper "On Characterization of molecular branching". Zagreb indices are one of the oldest degree-based topological indices in analyzing the structuredependence of total π-electron energy. Neighborhood degree is the summation of the degree of the nearest(neighborhood) vertices and is denoted as S_u whereas the degree of a vertex is the number of edges meet at the vertex u and is denoted as d_u.

In chemical applicability, many degree-based as well as neighborhood degree-sum based topological indices are employed. It began in 1947 when the Wiener index was used to determine the physical properties of alkanes. One of the main applications of topological indices is to predict[19] the Physico-chemical properties of chemical compounds. Here we compare the predicting ability of the existing degree-based topological indices and their corresponding neighborhood degree-sum based topological indices like QSPR models to predict the properties[18] (boiling point- ***BP***, entropy-***S***, acentric factor, enthalpy of vaporization-***HVAP***, standard enthalpy of vaporization-***DHVAP***) of octane isomers.

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Preliminaries

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Throughout this paper, we have taken molecular graph G where the vertex set contains the atoms as vertices and edge set contains connectors(bonds) as edges.

Degree $d_u(G)$is considered as $d_u(G) = \{u \epsilon V(G) / uv \epsilon E(G)\}$

Neighborhood degree-sum $S_u$is considered as

$S_u(G) = \sum_{u \epsilon N(G)} d_u$ where $N(G)$ is the set of neighborhood vertices of u.

Table 1 shows the basic definitions of degree-based & their corresponding neighborhood-degree-based topological indices.

No	Degree-based topological indices	Neighborhood degree-sum topological indices
1	[7] Augmented Zagreb Index $Az(G) = \sum_{u,v \in E} \left(\frac{d_u d_v}{d_u+d_v-2}\right)^3$	[13] Sanskruti Index $S(G) = \sum_{u,v \in E} \left(\frac{S_u S_v}{S_u+S_v-2}\right)^3$
2	[2] Atom Bond Connectivity Index $ABC(G) = \sum_{u,v \in E} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$	Fourth version of Atom Bond Connectivity Index $ABC_4(G) = \sum_{u,v \in E} \sqrt{\frac{S_u+S_v-2}{S_u S_v}}$
3	[16] Geometric Arithmetic Index $GA(G) = \sum_{u,v \in E} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$	Fifth version of Geometric Arithmetic Index $GA_5(G) = \sum_{u,v \in E} \frac{2\sqrt{S_u S_v}}{S_u+S_v}$
4	Harmonic Index $H(G) = \sum_{u,v \in E} \frac{2}{d_u+d_v}$	[17] Neighborhood version of Harmonic Index $NH(G) = \sum_{u,v \in E} \frac{2}{S_u+S_v}$
5	[12] Forgotten Index $F(G) = \sum_{u,v \in E} (d_u)^2 + (d_v)^2$ Or $F(G) = \sum_{u \epsilon V} (d_u)^3$	[17] Neighborhood version of Forgotten Index $NF^*(G) = \sum_{u,v \in E} (S_u)^2 + (S_v)^2$ and $NF(G) = \sum_{u \epsilon V} (S_u)^3$
6	[5] First Zagreb Index $M_1(G) = \sum_{u,v \in E} d_u + d_v$ Or $M_1(G) = \sum_{u \epsilon V} (d_u)^3$	[17] Neighborhood version of First Zagreb Index $NM_1^*(G) = \sum_{u,v \in E} S_u + S_v$ and $NM_1(G) = \sum_{u \epsilon V} (S_u)^2$
7	[5] Second Zagreb Index $M_2(G) = \sum_{u,v \in E} d_u d_v$	[17] Neighborhood version of Second Zagreb Index$NM_2(G) = \sum_{u,v \in E} S_u S_v$
8	[3] *Randic Index* $R(G) = \sum_{u,v \in E} \frac{1}{\sqrt{d_u d_v}}$	Neighborhood version of Randic Index $NR(G) = \sum_{u,v \in E} \frac{1}{\sqrt{S_u S_v}}$
9	[3] Sum Connectivity Index $S(G) = \sum_{u,v \in E} \frac{1}{\sqrt{d_u+d_v}}$	Neighborhood version of Sum Connectivity Index $NS(G) = \sum_{u,v \in E} \frac{1}{\sqrt{S_u+S_v}}$
10	[10] Hyper Zagreb Index$HM(G) = \sum_{u,v \in E} (d_u + d_v)^2$	[17] Neighborhood version of Hyper Zagreb Index $NHM(G) = \sum_{u,v \in E} (S_u + S_v)^2$

Table 2 and 3 show the results of the ten degree-based topological indices and their corresponding neighborhood degree-sum degree based topological indices. Forgotten Index

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and First Zagreb Index are calculated by vertex as well as edge partition methods. Their corresponding neighborhood degree-sum topological indices($NF^*(G) \neq NF(G)$ &$NM_1^*(G) \neq NM1(G)$) give unequal values. Table 4 shows the results of correlation between the basic Physico-chemical properties(*BP*,*S*, Acentric factor, *HVAP & DHVAP*) of n-octane isomers with mentioned degree-based as well as neighborhood degree-based topological indices.

Table 2. Shows the results of degree-based topological indices with n-octane isomers

Octane isomers	*Az*(*G*)	*ABC*(*G*)	*GA*(*G*)	*H*(G)	*F*(*G*)	$M_1(G)$	$M_2(G)$	*R*(*G*)	*SUM*(*G*)	*HM*(*G*)
	56	4.94977	6.88562	3.83333	50	26	24	3.91422	3.6547	98
	46.75	5.16855	5.67486	3.56667	62	28	26	3.77006	3.52456	114
	51.375	5.05916	6.71124	3.63334	62	28	27	3.80807	3.54912	116
	51.375	5.05916	6.71124	3.63334	62	28	27	3.80807	3.54912	116
	56	4.94977	6.76782	3.7	62	28	28	3.84608	3.57368	118
	39.1111	5.42653	6.28562	3.2	92	32	30	3.56067	3.32723	152
	45.51563	5.2375	6.52069	3.4	74	30	30	3.68074	3.43281	134
	42.125	5.27794	6.43028	3.36667	74	30	29	3.66391	3.41898	132
	37.5	5.38733	6.42369	3.3	74	30	28	3.6259	3.39442	130
	44.74074	5.26761	6.37124	3.30006	92	32	32	3.62134	3.36562	156
	50.14063	5.12811	6.57726	3.20482	74	30	31	3.71875	3.45732	136
	50.14063	5.12811	6.57726	3.20482	74	30	31	3.71875	3.45732	136
	50.37037	5.10869	6.45686	2.73333	92	32	34	3.68201	3.40401	160
	40.31011	5.47431	6.17838	3.05238	104	34	35	3.48139	3.24415	174
	29.86111	5.64531	6.05466	2.93333	104	34	32	3.41651	3.19709	168
	41.31471	5.42478	6.70741	3.08571	104	34	36	3.50405	3.25798	176
	39.65626	5.41584	6.33012	3.16667	86	32	33	3.55342	3.3165	152
	33.18518	5.80855	5.8	2.65	134	38	40	3.25	3.03682	214

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Table 3. shows the results of neighborhood-degree-based topological indices with n-octane isomers

Octane isomers	*S*	ABC_4	GA_5	*NH*	*N*F*	*NF*	*N* M_1*	*N M_1*	*N M_2*	*NR*	*NSUM*	*N HM*
	100.537	4.54233	6.93908	2.12143	172	326	48	90	84	2.14386	2.71099	340
	115.0822	4.4392	6.93664	1.95158	202	406	52	104	98	1.97151	2.60130	398
	122.61378	4.44109	6.86822	1.91348	224	448	54	108	106	1.9559	2.56987	436
	123.91016	4.44298	6.86435	1.95000	228	472	54	110	107	1.9911	2.58753	442
	124.14258	4.45621	6.78913	1.89849	252	520	56	114	115	1.96436	2.55123	482
	155.83184	4.25251	6.92663	1.73420	274	632	60	138	132	1.75445	2.44290	538
	145.952	4.32354	6.81908	1.73586	282	582	60	126	129	1.78369	2.44421	540
	138.63364	4.34725	6.86001	1.75880	258	558	58	124	121	1.79941	2.46879	500
	132.46078	4.33091	6.94658	1.78730	232	486	56	118	113	1.80194	2.49494	458
	170.69576	4.2673	6.78158	1.65642	220	728	64	146	148	1.71766	2.38115	620
	150.66144	4.34319	6.73084	1.67778	306	630	62	130	136	1.75341	2.40431	578
	163.11248	4.31513	6.56525	1.63417	330	727	64	141	146	1.71322	2.37217	622
	182.73748	4.29184	6.40313	1.53896	374	806	68	152	163	1.64476	2.30143	700
	192.86378	4.13509	6.75786	1.46900	384	850	70	162	171	1.52741	2.25203	726
	170.60628	4.1673	6.83317	1.58659	312	778	64	156	147	1.6062	2.34610	606
	200.76881	4.1345	6.62052	1.41431	408	874	72	164	179	1.48892	2.21368	766
	166.33789	4.21608	6.60986	1.53333	342	728	66	144	151	1.58908	2.30779	644
	248.75879	3.89657	6.77254	1.23377	488	1070	80	194	217	1.27674	2.07632	922

Comparative Analysis

(a) Between degree-based & neighborhood degree-based topological indices in correlation with Physico-chemical properties of n-octane isomers.

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(b) Between Augmented Zagreb Index with Atom-bond Connectivity Index based on the correlation with boiling point of octane isomers.

(a) Based on the results shown in table 2 & 3, the ten degree-based topological indices and their corresponding twelve neighborhood degree-based topological indices are correlated with the basic Physico-chemical properties [19, 20]of n-octane isomers(Table 4).

Table 4. shows the results of correlation coefficients between the physicochemical properties of n-octane isomers with degree-based as well as neighborhood degree-sum based topological indices.

Topological Index	*BP*	*S*	Acentric Factor	*HVAP*	*DHVAP*
$Az(G)$	0.9223	0.6863	0.6676	0.9378	0.8997
$S(G)$	-0.5352	-0.9556	-0.9844	-0.7504	-0.831
$ABC(G)$	-0.8631	-0.8207	-0.7929	-0.9298	-0.9253
$ABC_4(G)$	0.6998	0.953	0.9594	0.8611	0.913
$GA(G)$	0.5964	0.5219	0.4425	0.6440	0.5911
$GA_5(G)$	-0.1126	0.4389	0.5518	0.1529	0.2317
$H(G)$	0.6154	0.9124	0.9253	0.8121	0.8577
$NH(G)$	0.5696	0.9334	0.9857	0.7844	0.8520
$F(G)$	-0.7047	-0.9528	-0.965	-0.8716	-0.924
$NF^*(G)$	-0.398	-0.8888	-0.9227	-0.6287	-0.7135
$NF(G)$	-0.5493	-0.9300	-0.9912	-0.7636	-0.8412
$M_1(G)$	-0.7203	-0.9543	-0.9731	-0.886	-0.9361
$NM_1^*(G)$	-0.4951	-0.9361	-0.9850	-0.7222	-0.8063
$NM_1(G)$	-0.6235	-0.9475	-0.9947	-0.8181	-0.8875
$M_2(G)$	-0.5007	-0.9410	-0.9864	-0.7281	-0.8118
$NM_2(G)$	-0.4955	-0.9427	-0.9844	-0.7191	-0.8063
$R(G)$	0.8208	0.9061	0.9042	0.9361	0.9582
$NR(G)$	0.6326	0.9456	0.9839	0.8300	0.8881
$SUM\ (G)$	0.8023	0.9231	0.9299	0.9318	0.9612
$NSUM(G)$	0.5517	0.9364	0.9879	0.7699	0.8881
$HM(G)$	-0.6567	-0.9613	-0.9829	-0.8425	-0.9043
$NHM(G)$	-0.4591	-0.9319	-0.9787	-0.6917	-0.7818

From the following paragraphs, predictive ability[22,23] of the above mentioned ten topological indices and their corresponding twelve neighborhood degree-sum topological

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indices are tested with basic Physico-chemical properties of eighteen structural octane isomers are discussed.

Boiling Point(*BP*) Augmented Zagreb Index and Atom Bond Connectivity Index show higher correlation(0.9223 & 0.8631) than other degree based topological indices. Besides their corresponding neighborhood degree-based topological indices show moderated correlation withboiling point of n-octane isomers. The important analysis regarding the correlation, degree based topological indices are higher than their corresponding neighborhood-degree-based topological indices.

Entropy(*S*) Sanskruti Index (neighborhood degree based topological index of Augmented Zagreb Index) shows higher value(|0.9553|) than Augmented Zagreb Index. In the same way, ABC_4 Index, *NH* index, NM_2 index, *NR* index &*NSUM* index express higher correlation with entropy of n-octane isomers than their corresponding degree-based topological indices.

Acentric Factor This propertyof n-octane isomers is highly correlated with neighborhood degree-sum of the above-mentioned topological indices than their corresponding degree-based indices except neighborhood version of Hyper Zagreb Index & Second Zagreb Index (considerably insignificant deviation).

HVAP&DHVAP This correlation coefficients linking the *HVAP&DHVAP* of n-octane isomers and mentioned degree based topological indices exhibit higher value than their corresponding neighborhood version of degree-based indices. It indicates that, degree-based topological indices should be preferred in designing quantitative structure-property relations with the above Physico-chemical properties of n-octane isomers.

(b) Generalized formulation of Augmented Zagreb Atom Bond Connectivity Index

$$(\mathrm{AzABC})_\alpha(G) = \sum_{u,v \in E} \left(\frac{d_u\, d_v}{d_u + d_v - 2}\right)^\alpha \quad \text{where } \alpha \epsilon \mathrm{R}$$

When $\alpha = 3$, $Az(G) = \sum_{u,v \in E} \left(\frac{d_u\, d_v}{d_u + d_v - 2}\right)^3$ and $\alpha = -1/2$, $ABC(G) = \sum_{u,v \epsilon E} \sqrt{\frac{d_u + d_v - 2}{d_u\, d_v}}$

The interesting factor of these two indices is that they show higher correlation value than other degree-based indices with boiling point of n-octane isomers. This feature leads us to investigate with numerous values of α to get comparatively good correlation for further studies.

Table 5. shows correlation coefficients of boiling point of n-octane isomers with the indices.

α	$\lvert(\mathrm{AzABC})_\alpha(G)\rvert$
1	0.887
2	0.9042

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3	0.9223 *Az*(*G*)
-1/3	0.8656
-1/2	0.8631 *ABC*(*G*)
-1	0.8564
-2	0.8434

From the results of Table 5 reveal that, when α is positive, the correlation of boiling point of n-octane isomers high with increasing α values and at the same time α is negative, the correlation decreased with decreasing α values.

Conclusion

From the above results, we conclude that degree-based topological indices are more suitable than neighborhood degree-sum topological indices in the predictive study of boiling points of structural isomers. Among the indices Augmented Zagreb Index and Atom Bond Connectivity Index are suitable for structure property relations linked with boiling points of n-octane isomers. *HVAP* and *DHVAP* of isomers are highly correlated with neighborhood degree-sum topological indices. This paper will pave the path for many intricate predictive analyses of structural isomers for their chemical applications.

Table 6. Shows the of experimental values[18] of boiling point, entropy, acentric factor, enthalpy of vaporization & standard enthalpy of vaporization of eighteen structural octane isomers.

S. No	Octane isomers	BP	S	Acentric Factor	HVAP	DHVAP
1	n-octane	125.665	111.67	0.397898	73.19	9.915
2	2-methyl heptane	117.647	109.84	0.377916	70.30	9.484
3	3-methyl heptane	118.925	111.26	0.371002	71.3	9.521
4	4-methyl heptane	117.709	109.32	0.371504	70.91	9.483
5	3-ethyl hexane	118.534	109.43	0.362472	71.70	9.476
6	2,2-dimethyl hexane	106.840	103.42	0.339426	67.70	8.915
7	2,3-dimethyl hexane	115.607	108.02	0.348247	70.20	9.272
8	2,4-dimethyl hexane	109.429	106.98	0.344223	68.50	9.029
9	2,5-dimethyl hexane	109.103	105.72	0.356830	68.60	9.051
10	3,3-dimethyl hexane	111.969	104.74	0.322596	68.50	8.973
11	3,4-dimethyl hexane	117.725	106.59	0.340345	70.20	9.316
12	2-methyl-3-ethyl pentane	115.450	106.06	0.332433	69.70	9.209
13	3-methyl-3-ethyl pentane	118.259	101.48	0.306899	69.30	9.081
14	2,2,3-trimethyl pentane	109.841	101.31	0.300816	67.30	8.826
15	2,2,4-trimethyl pentane	99.238	104.09	0.305370	64.87	8.402
16	2,3,3-trimethyl pentane	114.760	102.06	0.293177	68.10	8.897
17	2,3,4-trimethyl pentane	113.467	102.39	0.317422	68.37	9.014
18	2,2,3,3-tetramethyl butane	106.470	93.06	0.255294	66.20	8.410

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