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Apposite degree-Based Topological Indices are the Predicting Tools for the Physico-Chemical Properties of Structural Isomers

A Running title: Apposite Degree-Based Topological Indices are the Predicting Tools for the Physico-Chemical Properties of Structural Isomers

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ABSTRACT

In this paper, twenty existing degree-based topological indices are selected and computed with twelve structural isomers of C_9H_{18}containing cyclohexane ring. The results of all these topological indices are correlated with the Physico-chemical properties such as the boiling point, vapor pressure, and enthalpy of vaporization of the above-mentioned isomers. The way forward, correlation coefficients of isomeric octanes[1] for same topological indices with same properties numbered and compared.

Keywords: Topological indices, cyclohexane, isomers, correlation coefficient, QSAR, QSPR.

Introduction

A molecular graph is a collection of points in lieu of atoms in the molecule and a set of line s for covalent bonds. In graph theory, these points are name dvertices and the lines are named edges. A topological index is a number associated with the vertex set and the edge set of the graph *G* (*V*, *E*). And are gene rally classified into three kinds, degree-based indices, distance-based indices, and spectrum-based indices. Few topological indices are based on both degrees and istances.

Some topological indices help in predicting the Physico-chemical properties and representing in quantitative structure-activity/structure-property relationship (QSAR, QSPR) modeling. These numbers of indices have been predictably used in QSAR/QSPR studies for drug discovery and design in medical chemistry. The degree-based topological index–Augmented index plays an important role in predicting the boiling points of the structural isomers and will be using in a QSPR model for seeing their structural properties.

The biopharmaceutical industry is at a peak point in terms of recalibration. Companies are progressively looking to use big data and predictive analysis to improve R&D productivity. Any method supporting electing the structure worth of being synthesized and tested will affect incredible savings.

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Precisely, boiling point and vaporpres sure are influenced by inter-molecular and van-der-walls kind interaction. In this article, we computed the twenty well established degree-based topological indices and found the correlationco efficients of the indices with the Physico-Chemical properties of the twelve structural isomers of C_9H_{18} containing cyclohexane ring. The accuracy level of topological indices is evaluated (regardless of isomer class) with some thermal properties. This article is especially focused on thermal property correlation and the top five topological indices showing[1] the accurate relationship among the isometric groups.

Basic Definitions

A molecular graph G of hydrocarbons is hydrogen depicted and has the ultimate degree of vertices 4. The first degree-based topological index was set forth[2] in 1975 by Milan Randic has been studied expansively by both Chemists and Mathematicians due to its applicability in chemistry. This index is defined as

$$R_{-1/2}(G) = \sum_{u,v \in E} \frac{1}{\sqrt{d_u d_v}}$$

Generalized Randi*ć*index is framed in the place of ½ has replaced by δ[4](numerical values other than – ½) in Randi*ć* index gives an infinite number of topological indices of the form

$$R_{\delta}(G) = \sum_{u,v \in E} [d_u\, d_v]^{\delta}$$

In this article, δ = ½, -1 valued indices [$R_{½}(G)$, $R_{-1}(G)$]are calculated.

In addition to that Reduced Reciprocal Randi*ć* index[6] is calculated for the 12 structural isomers of

C_9H_{18} containing cyclohexane ring.

This index was defined as

$$RRR(G) = \sum_{u,v \in E} \sqrt{(d_u - 1)(d_v - 1)}$$

The sum connectivity index[7], which was introduced by Zhou and Trinajsti*ć* in 2008. It is a newindex closelyassociated *to the* Randi*ć*(product-connectivity)index.

This index was defined as

$$S(G) = \sum_{u,v \in E} \frac{1}{\sqrt{(d_u + d_v)}}$$

Ivan Gutman *et al* introduced the first Zagreb index and second Zagreb index[9] followed by G.H. Fath-Tabar *et al* introduced third Zagreb index[10] and were defined here as

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$M_1(G) = \sum_{u \in V}(d_u)^2$ or $M_1(G) = \sum_{u,v \in E}(d_u + d_v)$

$M_2(G) = \sum_{u,v \in E} d_u . d_v$

$M_3(G) = \sum_{u,v \in E} | d_u - d_v |$

The redefined version of Zagreb indices(1,2,3) is introduced by Ranjini *et al* and are demarcated as

$ReZ_1(G) = \sum_{u,v \in E} \frac{d_u . d_v}{d_u + d_v}$

$ReZ_2(G) = \sum_{u,v \in E} \frac{d_u + d_v}{d_u . d_v}$

$ReZ_3(G) = \sum_{u,v \in E}(d_u + d_v)(d_u . d_v)$

Above mentioned Zagreb indices are comparatively inadequate for any structure-property correlation. The indices such as Reduced Second Zagreb index[12], First Hyper Zagreb index[13], second Hyper Zagreb index[13]& Augmented Zagreb index are also playing important role in the molecular chemistry field.

And they were defined as

$RM_2(G) = \sum_{u,v \in E}(d_u - 1)(d_v - 1)$

$HM_1(G) = \sum_{u,v \in E}(d_u + d_v)^2$

$HM_2(G) = \sum_{u,v \in E}(d_u . d_v)^2$

$AZ(G) = \sum_{u,v \in E} \left(\frac{d_u . d_v}{d_u + d_v - 2}\right)^3$

Augmented Zagreb index which was introduced by Furtula *et al*[12], gives high correlation of structural isomers with their structural properties.

Estrada *et al* introduced atom bond connectivity index which significantly good in Physico-Chemical properties and it was denoted as

$ABC(G) = \sum_{u,v \in E} \left(\sqrt{\frac{d_u + d_v - 2}{d_u . d_v}}\right)$

Harmonic index[14,15] and Geometric Arithmetic index[16] are also having collectively good

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correlation with the structural isomers and their physicochemical properties & were defined as

$$H(G) = \sum_{u,v \in E} \frac{2}{d_u + d_v}$$

$$GA(G) = \sum_{u,v \in E} \left(\frac{2\sqrt{d_u . d_u}}{d_u + d_v} \right)$$

Furtula and Gutman have reformulated the Forgotten index[17] which was highly connect with new drug's medical and biological contents and was defined as

$$F(G) = \sum_{u \in V} (d_u)^3 \quad \text{or}$$

$$F(G) = \sum_{u,v \in E} (d_u)^2 + (d_v)^2$$

Main Results and Comparative Analysis

Here, twenty degree-based topological indices of structural isomers of C_9H_{18}containing cyclohexane ring calculated and listed in Table 2 & Table 3.

The Physico-chemical properties[21] such as boiling point (*bp* ℃), vapor pressure (*Vp mmHg at* 25℃), and enthalpy of vaporization (Δ*Hvap)* of the mentioned isomers are correlated with the mentionedtopologicalindices.Theresultsaredisplayedin Table6.Correlationcoefficientsof the boiling point of the isomers with the five among the twenty indices are pretty high and the interesting factor that these five indices are reaching a high correlation with n-octane isomers[1]. The comparison is exhibited in Table4.

Table 1. displays the twelve structural isomers of C_9H_{18}containing cyclohexane ring.

Table 1

1,3,5 Trimethyl cyclohexane		1,3,3Trimethyl cyclohexane		1 ethyl 3 methyl cyclohexane	
1,2,3 Trimethyl cyclohexane		1,1,4Trimethyl cyclohexane		1 ethyl 4 methyl cyclohexane	
1,2,4 Trimethyl cyclohexane		1 ethyl 1 methyl cyclohexane		Iso methyl cyclohexane	
1,2,2Trimethyl cyclohexane		1 ethyl 2 methyl cyclohexane		Propyl cyclohexane	

Table 2&3. shows the outcomes of the twenty topological indices with the structural isomers of C_9H_{18}containing cyclohexane ring.

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Table 2

Isomers	$R_{1/2}$	R_{-1}	*RR*	*RRR*	*S*	M_1	M_2	M_3	ReZ_1	ReZ_2	ReZ_3
1,3,5 Trimethyl cyclohexane	4.18154	2	19.89309	8.48528	4.18328	42	45	12	9.45	9	216
1,2,3 Trimethyl cyclohexane	4.21522	2.0556	20.09513	8.82843	4.0611	42	47	8	9.65	9	200
1,2,4Trimethyl Cyclohexane	4.19837	2.02778	19.99915	8.65685	4.1971	42	46	10	9.55	9	226
1,2,2 Trimethyl Cyclohexane	4.12783	1.95833	20.47408	8.59575	4.12784	44	49	12	9.59762	9	262
1,3,3 Trimethyl Cyclohexane	4.10096	1.91667	20.28788	8.29253	4.10535	44	47	14	9.41667	9	240
1,1,4 Trimethyl Cyclohexane	4.10096	1.91667	20.28788	8.29253	4.10535	44	47	14	9.41667	9	240
1 ethyl 1 methyl Cyclohexane	4.26777	2.125	18.76268	9.19615	4.24931	42	46	10	9.46667	9	234
1 ethyl 2methyl Cyclohexane	4.34252	2.19444	19.49473	9.24264	4.32724	40	44	6	9.51667	9	210
1 ethyl 3 methyl Cyclohexane	4.3257	2.16667	19.3971	9.07107	4.31342	40	43	8	9.16667	9	200
1 ethyl 4 methyl Cyclohexane	4.3257	2.16667	19.3971	9.07107	4.31342	40	43	8	9.16667	9	200
Isopropyl Cyclohexane	4.30453	2.11111	19.86308	8.82843	4.30268	40	43	6	9.4	9	202
Propyl Cyclohexane	4.43185	2.25	18.76268	9.24264	4.41899	38	40	4	9.26667	9	176

Table 3

Isomers	RM_2	HM_1	HM_2	*AZ*	*H*	*ABC*	*GA*	*F*	*SDD*
1,3,5 Trimethyl cyclohexane	12	198	243	58.125	3.9	6.69214	8.47686	108	23
1,2,3 Trimethyl cyclohexane	14	202	293	64.90625	3.74444	6.61125	8.55767	108	18.3333
1,2,4Trimethyl Cyclohexane	13	200	268	61.51563	3.93333	6.6517	8.51726	108	20.66667

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1,2,2 Trimethyl Cyclohexane	14	224	333	61.93974	3.81904	6.72958	8.37838	126	19.5
1,3,3 Trimethyl Cyclohexane	12	220	273	56.11574	3.76667	6.7912	8.31182	126	20.16667
1,1,4 Trimethyl Cyclohexane	12	220	273	56.11574	3.76667	6.7912	8.31182	126	20.16667
1 ethyl 1 methyl Cyclohexane	13	206	276	66.37037	4.06667	6.52288	8.1923	114	18.25
1 ethyl 2methyl Cyclohexane	13	184	250	70.76563	4.2	6.43292	8.74823	96	16.33333
1 ethyl 3 methyl Cyclohexane	12	182	225	67.375	4.16667	6.47335	8.70782	96	18.7777
1 ethyl 4 methyl Cyclohexane	12	182	225	67.375	4.16667	6.47335	8.70782	96	18.7777
Isopropyl Cyclohexane	12	182	235	66.14063	4.13333	6.5423	8.69164	96	16
Propyl Cyclohexane	11	164	192	72	4.36667	6.36936	8.8822	84	14

Table 4. shows the comparison between the correlation coefficients of five topological indices with structural isomers of C_9H_{18} containing cyclohexane ring & eighteen n-octane structural isomers.

Table 4

Topological indices	Isomers of $C_9H_{18}$with cyclohexane	Isomers of n-octane
AZ	0.9401	- 0.922
ABC	-0.9245	0.890
RRR	0.9267	0.8776
R_{-1}	0.9187	-0.886
R	-0.9107	-0.846

Table 5. shows the values[21] of *bp*℃, *VpmmHg* at 25℃&ΔH_{vap}*KJ/mol* of twelve structural isomers of C_9H_{18} cyclohexane ring.

Table 5

Isomers of C_9H_{18} with cyclohexane	*bp*℃	*VpmmHg* at 25℃	ΔH_{vap}*KJ/mol*
1,3,5 Trimethyl cyclohexane	139.5	8.0	36.1
1,2,3 Trimethyl cyclohexane	143.5	6.7	36.5
1,2,4Trimethyl Cyclohexane	143.5	6.7	36.5
1,2,2 Trimethyl Cyclohexane	145.2	6.2	36.6
1,3,3 Trimethyl Cyclohexane	138.5	8.3	36
1,1,4 Trimethyl Cyclohexane	135	9.7	35.7

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1 ethyl 1 methyl Cyclohexane	152.2	4.5	37.3
1 ethyl 2methyl Cyclohexane	150.8	4.8	37.2
1 ethyl 3 methyl Cyclohexane	150.8	4.8	37.2
1 ethyl 4 methyl Cyclohexane	150.8	4.8	37.2
Isopropyl Cyclohexane	151.9	4.6	37.3
Propyl Cyclohexane	155.8	3.8	37.6

Table 6. displays the correlation between structural properties such as *bp*, *Vp*&ΔH_{vap} with the twelve structural isomers of C_9H_{18} and the twenty topological indices.

Table 6

*TI*s	*bp*(◦C)	*Vp* (mm Hg at 25◦C)	ΔH_{vap}
R	-0.9107	- 0.887	0.9163
R_{-1}	0.9187	-0.9022	0.9255
RR	-0.7958	0.7575	-0.7948
RRR	0.9267	- 0.9232	0.4535
S	0.8574	-0.8214	0.8598
M_1	-0.8344	0.8093	-0.8416
M_2	-0.7076	0.6592	-0.7129
M_3	-0.866	0.8562	-0.8723
Re Z_1	-0.4018	0.3533	-0.4091
Re Z_2	NaN	NaN	NaN
Re Z_3	-0.5935	0.56667	-0.6044
R M_2	-0.164	0.0846	0.1633
HM_1	-0.7728	0.7473	-0.7815
HM_2	-0.5121	0.4621	-0.5257
AZ	0.9401	-0.9350	0.6054
H	0.8900	-0.8559	0.6469
ABC	-0.9245	0.9084	-0.6076
GA	0.6217	-0.6111	0.8764
F	-0.781	0.7671	-0.7399
SDD	-0.7935	0.7543	-0.7906

Conclusion

Twenty degree-based topological indices of structural isomers C_9H_{18} containing cyclohexane ring are calculated and tabled (Tables 1 & 2). The three primary thermal properties like vapor pressure, boiling point, and enthalpy of vaporization with the twenty topological indices of isomers correlation coefficients are evaluated and tabled(Table 5). The correlation

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coefficients of the boiling point of the structural isomers of C_9H_{18} containing cyclohexane ring with eighteen structural octane isomers are compared and tabled(Table 3).

Remarkably Augmented Zagreb topological index[1] is showing a precise correlation with both isomers group with all three primary thermal properties. Atom Bond Connectivity index, Reduced Reciprocal Randić index, Randić indices R_{-1}, $R_{1/2}$ are also giving significant correlation in both isomer groups.

This opens up further many explorations as other structural isomers correlate to Augmented Zagreb topological index and the remaining four indices mentioned in the previous paragraph.

Relative atoms position affects the thermal properties of isomers. This is the area to explore, Augmented Zagreb topological index is exactly suitable for finding the relative position of atoms and the possibility to arrive at further precise results from the baseline of this topological index.

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