

On Van Molecular Topological Modelling of Fullerenes' Chemical Properties

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Abstract: In addition to graphite, diamond, and nanotubes, fullerenes are a fundamental allotrope of carbon that has received significant attention in the fields of nanoscience, nanotechnology, condensed matter physics and chemistry, biological physics, materials science and technology, mechanical and electrical sciences, biomedical engineering, and most recently, medical nanotechnology and nano-neuroscience. Molecular topological indices are essential tools to relate the theoretical and physical properties of chemical substances. Investigation of the chemical and physical properties of fullerenes' topological indices has been started in recent years. This study presents topological modelling of fullerenes' binding energies, the heat of formation, shape resonances, and Ramsauer-Townsend minima using the Van molecular topological index.

Keywords: fullerenes; topological analysis; topologic index; Van index.

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1. Introduction

Over the past few decades, nanomaterials based on carbon have evolved quickly. These include fullerenes, carbon nanotubes, graphene and its derivatives, graphene oxide, nanodiamonds, and carbon-based quantum dots. Due to their distinct chemical and physical characteristics, which offer significant potential in various applications, fullerenes have stood out among them and have drawn increased scientific attention [1]. Since Kroto et al.'s first discovery of fullerene (buckyball), many carbon-based and inorganic (non-carbon-based) nanostructures have been assessed for their potential use in photovoltaics, corrosion control, storage of energy, gas sensing, and drug sensitivity [2-11]. Chemical graph theory uses graphs to mathematically represent chemical structures. In chemical graph theory and mathematical chemistry, a chemical graph is a graph-theoretic representation of the structural formula of a compound. Atoms are shown as vertices, and atomic bonds are shown as edges in the chemical graph. A molecular structure descriptor that describes the topology of the compound is a topological index, also known as a connectivity index [12,13]. Topological indices are essential tools to relate the theoretical and physical properties of chemical substances. To detect the quantitative structure analysis of chemicals, nanostructures, and pharmaceuticals, degree-based topological indices (TIs) are helpful [14-20].

Quantum molecular dynamics (QMD) has been used to examine the compressive mechanical characteristics of fullerene molecules. It is possible to determine the fullerene molecules' compressive stiffness, endurance load, failure strain corresponding to the endurance load, and energy- and force-strain curves [21]. The degree-based topological indices can be used to display the physical characteristics of fullerenes [22-25]. The atom-bond connectivity (ABC) and geometric-arithmetic (GA) indices of fullerene networks and carbon nanotube networks were examined as two degree-based topological indices [22]. For all isomers of tiny (5,6)-fullerenes, a collection of ZZ polynomials—also known as Zhang–Zhang polynomials or Clar covering polynomials—was presented in ref. [23]. The results that have been presented should be valuable as benchmark information for creating algorithms and computer programs that analyze "fullerenes' topology and create resonance structures for calculations involving valence bonds in quantum chemistry [23]. Based on molecular topological indices such as the Szeged index (Sz), Mostar index (Mo), PI-index (PI), Wiener and hyper Wiener (WW) indices, which are computed from distance matrices, have been reported topological peripheral shape and distance-based distance estimates of 82 fullerene cages [23]. Also, the novel idea of isoperipheral fullerene cages as a result of the new results for the Mo, Sz, and PI indices of these cages, which show the presence of both isomeric and non-isomeric fullerene cages with the same non-zero Mo indices, was introduced [24]. Well-known topological indices include the Randic, first and second Zagreb indices, and sum-based atomic bond connectivity indices have been calculated for the regression relations relating to the physical properties of fullerenes [25].

Among the significant physical characteristics of fullerenes are their binding energies (BE), Ramsauer-Townsend minima (RT minima), shape resonances (SR), and heat of formation (HoF). The BE is the quantity of energy required to separate a particle from a particle system or to scatter every particle present. Atomic nuclei, electrons linked to atomic nuclei, and atoms and ions bound together in crystals all serve as examples of the relevance of binding energy. The RT effect results from low-energy electrons being scattered by noble gas atoms. A potential 'barrier's shape traps an electron in the SR, a metastable situation. When a compound is produced from its component parts, each ingredient being in one mole, the amount of heat absorbed or evolved is known as the heat of formation (HoF). In 2017, Felfli and Msezane calculated these properties for fullerenes [26].

In this study, topological modeling of fullerenes' binding energies (BE), the heat of formation (HoF), shape resonances (SR), and Ramsauer-Townsend minima (RT) is presented by using the Van molecular topological index.

2. Materials and Methods

Let G be a chemical graph and v a vertex (atom) of G . The degree of vertex v , denoted as $\text{deg}(v)$, is the total number of edges which is incident to v . $N(v)$ is the set of all neighboring vertices of v . The sum degree of the vertex v , denoted as S_v , is the total number of all the degrees of neighboring vertices of v . The multiplication degree of the vertex v , denoted as M_v , is the sum of the total number of all the degrees of neighbouring vertices of v . The Van degree of the vertex v is defined as [27].

$$van(v) = \frac{S_v}{M_v} \quad (1)$$

Also, the reverse Van degree of the vertex v , defined as:

$$rvan(v) = \frac{M_v}{S_v} \quad (2)$$

Van topological indices are defined as [27]:

The first Van index of a simple connected graph G is defined as:

$$Van^1(G) = \sum_{v \in V(G)} van(v)^2 \quad (3)$$

The second Van index of a simple connected graph G is defined as:

$$Van^2(G) = \sum_{uv \in E(G)} van(u)van(v) \quad (4)$$

The third Van index of a simple connected graph G is defined as:

$$Van^3(G) = \sum_{uv \in E(G)} [van(u) + van(v)] \quad (5)$$

The first reverse Van index of a simple connected graph G is defined as:

$$Van^{1r}(G) = \sum_{v \in V(G)} rvan(v)^2 \quad (6)$$

The second reverse Van index of a simple connected graph G is defined as:

$$Van^{2r}(G) = \sum_{uv \in E(G)} rvan(u)rvan(v) \quad (7)$$

The third reverse Van index of a simple connected graph G is defined as:

$$Van^{3r}(G) = \sum_{uv \in E(G)} [rvan(u) + rvan(v)] \quad (8)$$

Every atom (vertex) of fullerene has degree three (Figure 1).

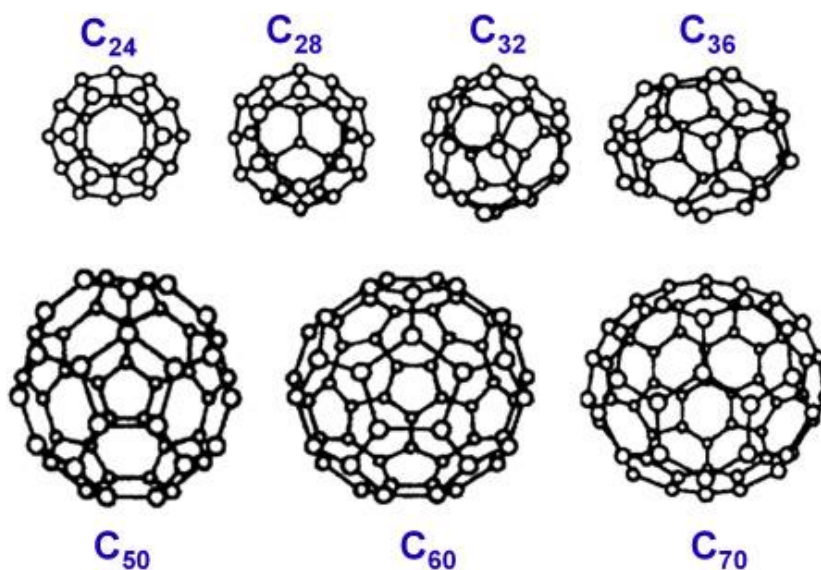


Figure 1. Some fullerene graphs.

3. Results and Discussion

Let G be a chemical graph of an n -vertex fullerene C_n and v be a vertex of C_n (In Figure 1, some fullerenes are shown). Table 1 shows the sum degree of v , the multiplication degree of v , and the Van degrees of v .

Table 1. Van degree values of any vertex v of fullerenes.

Notion	Symbol	Value
Sum degree	S_v	9
Multiplication degree	M_v	27
Van degree	$van(v)$	1/3
Reverse Van degree	$rvan(v)$	3

With the help of Table 1, we calculate and show six Van topological indices values of some fullerenes, following Tables 2-7.

Table 2. The first Van index $Van^1(C_n)$ values of some fullerenes.

Fullerene	Value	Fullerene	Value
C_{54}	6	C_{82}	9.111
C_{58}	6.444	C_{84}	9.333
C_{60}	6.666	C_{86}	9.555
C_{70}	7.777	C_{90}	10
C_{74}	8.222	C_{92}	10.222
C_{76}	8.444	C_{180}	20
C_{78}	8.666	C_{240}	26.666
C_{80}	8.888		

Table 3. The second Van index $Van^2(C_n)$ values of some fullerenes.

Fullerene	Value	Fullerene	Value
C_{54}	9	C_{82}	13.666
C_{58}	9.666	C_{84}	14
C_{60}	10	C_{86}	14.333
C_{70}	11.666	C_{90}	15
C_{74}	12.333	C_{92}	15.333
C_{76}	12.666	C_{180}	30
C_{78}	13	C_{240}	40
C_{80}	13.333		

Table 4. The third Van index $Van^3(C_n)$ values of some fullerenes.

Fullerene	Value	Fullerene	Value
C_{54}	54	C_{82}	82
C_{58}	58	C_{84}	84
C_{60}	60	C_{86}	86
C_{70}	70	C_{90}	90
C_{74}	74	C_{92}	92
C_{76}	76	C_{180}	180
C_{78}	78	C_{240}	240
C_{80}	80		

Table 5. The first reverse Van index $Van^{1r}(C_n)$ values of some fullerenes.

Fullerene	Value	Fullerene	Value
C_{54}	486	C_{82}	738
C_{58}	522	C_{84}	756
C_{60}	540	C_{86}	774
C_{70}	630	C_{90}	810
C_{74}	666	C_{92}	828
C_{76}	684	C_{180}	1620
C_{78}	702	C_{240}	2160
C_{80}	720		

Table 6. The second reverse Van index $Van^{2r}(C_n)$ values of some fullerenes.

Fullerene	Value	Fullerene	Value
C_{54}	729	C_{82}	1107
C_{58}	783	C_{84}	1134
C_{60}	810	C_{86}	1161
C_{70}	945	C_{90}	1215
C_{74}	999	C_{92}	1242
C_{76}	1026	C_{180}	2430
C_{78}	1053	C_{240}	3240
C_{80}	1080		

Table 7. The third reverse Van index $Van^{3r}(C_n)$ values of some fullerenes.

Fullerene	Value	Fullerene	Value
C_{54}	486	C_{82}	738
C_{58}	522	C_{84}	756
C_{60}	540	C_{86}	774
C_{70}	630	C_{90}	810

Fullerene	Value	Fullerene	Value
C ₇₄	666	C ₉₂	828
C ₇₆	684	C ₁₈₀	1620
C ₇₈	702	C ₂₄₀	2160
C ₈₀	720		

Surprisingly, the correlation efficiency between all six indices of fullerenes is one. Therefore, we conducted our analyses only for the first Van index values of fullerenes.

Some statistical techniques look into the interdependence between topological indices and the physical properties of molecules. The coefficient of correlation and regression analysis are two examples. Correlation measures the strength of the linkage, whereas linear regression employs an equation to express the linear relationship. The quantitative dependence of one variable on another is explained through regression. The percentage of data the regression line accurately represents is examined using the coefficient of determination.

The extent of a correlation is determined by the coefficient of correlation, which is described as the association between two or more variables that change in a particular direction. Since correlation describes how strongly two variables are associated, it is a symmetric relationship.

When two quantities A and B are correlated, then A and B are also correlated. Note that symmetrical relationships are not necessarily smooth. That is, variations in both variables occur simultaneously.

Linear relationships between SR, HoF, RT minima, BE of fullerenes, and the first Van index of fullerenes can be analyzed. We have collected these data from reference 26 for that purpose. Table 8 shows these characteristics.

Table 8. Physical properties of different fullerene structures, including heat of formation (HoF), binding energies (BE), the first and second shape resonances (SR), and the first and second Ramsauer-Townsend minima (RT).

Fullerene	BE (eV)	RT-1 (eV)	RT-2 (eV)	SR-1 (eV)	SR-2 (eV)	HoF (kcal/mol)
C ₅₄	3.14	0.94	2.92	0.08	1.28	642.0
C ₅₈	2.49	0.71	2.30	0.054	0.94	648.1
C ₆₀	2.66	0.76	2.46	0.061	1.02	618.1
C ₇₀	2.70	0.71	2.38	0.054	0.95	657.7
C ₇₄	3.21	0.82	2.68	0.068	1.1	694.6
C ₇₆	2.79	0.82	2.68	0.082	1.09	699.1
C ₇₈	2.98	0.87	2.85	0.068	1.16	712.5
C ₈₀	3.28	0.92	3.07	0.081	1.24	727.2
C ₈₂	3.15	0.95	3.06	0.081	1.26	727.8
C ₈₄	2.94	0.72	2.47	0.054	0.97	768.1
C ₈₆	2.92	0.75	2.58	0.054	1.0	745.7
C ₉₀	3.06	0.82	2.81	0.068	1.07	763.7

Regression analysis between individual physical properties, HoF, SR-1, SR-2, BE, RT-1, and RT-2, according to the first Van index (data in Table 8), can be illustrated by the following diagrams. A linear regression relationship can be derived from Figures 2-7 and Table 9. Most of the data points are fit by the heat of formation of the first Van index. The determined value of the coefficient is 0.8944, showing that it fits the observed values. Therefore, the regression line fits over 89% of the data. The first Van index and the heat of formation have a high positive connection, as indicated by the correlation coefficient of 0.9444.

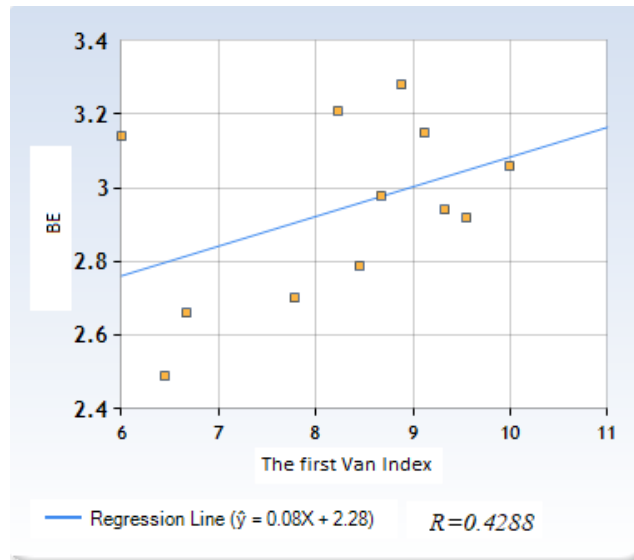


Figure 2. Analysis of BE based on the first Van index using regression.

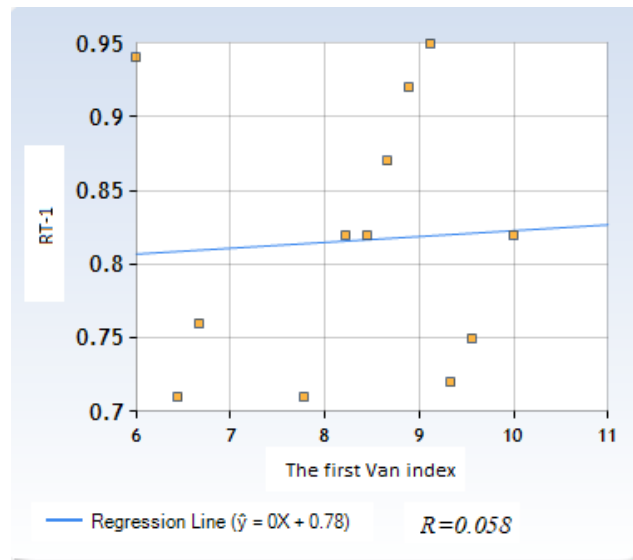


Figure 3. Analysis of RT-1 based on the first Van index using regression.

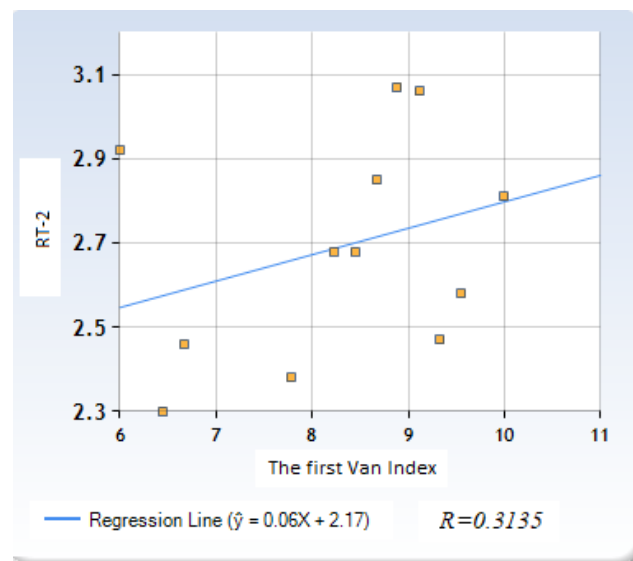


Figure 4. Analysis of RT-2 based on the first Van index using regression.

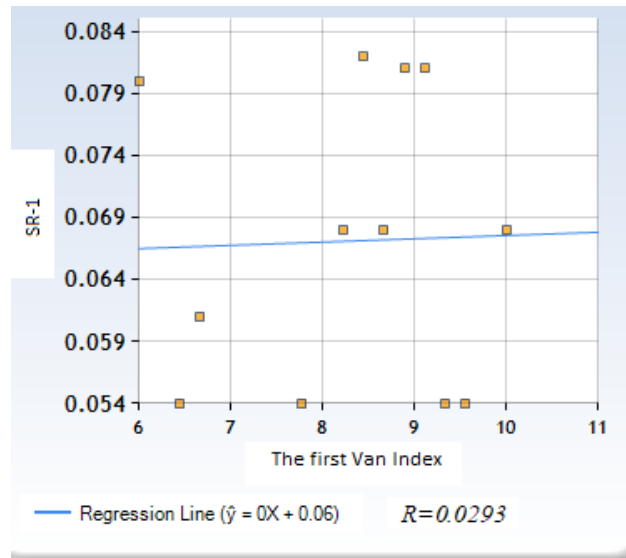


Figure 5. Analysis of SR-1 based on the first Van index using regression.

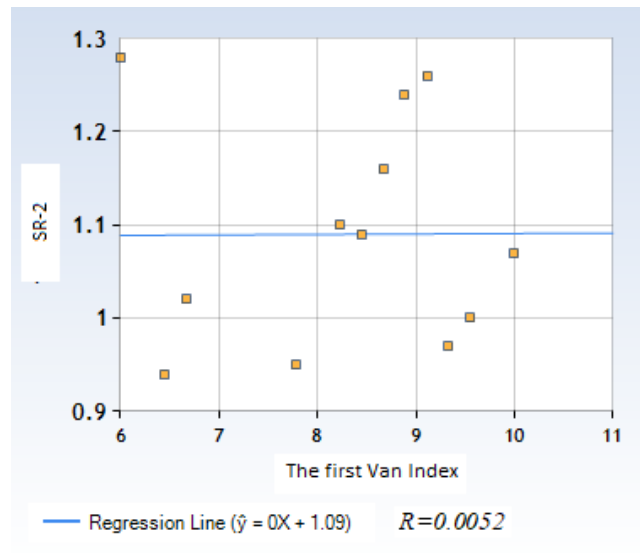


Figure 6. Analysis of SR-2 based on the first Van index using regression.

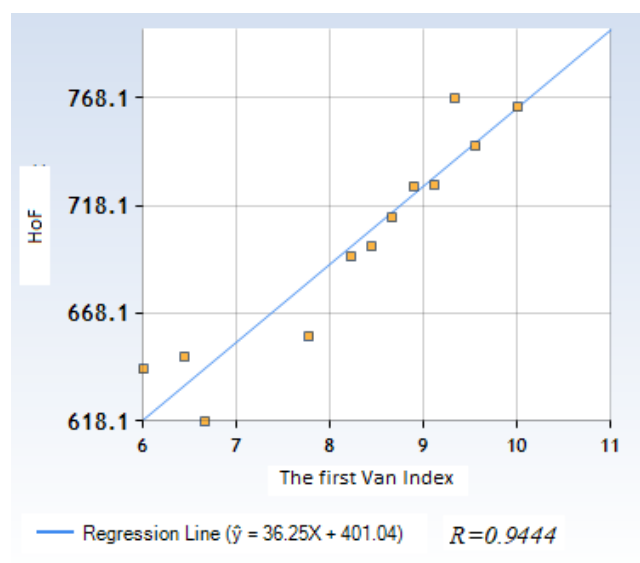


Figure 7. Analysis of HoF based on the first Van index using regression.

Table 9. Linear dependence relationships, Bes, HoF, RT-1, SR-1, RT-2, and SR-2 over fullerenes' first Van index values.

Property	Regression relation	Correlation (R)	Determination (R ²)
BE	$BE = 0.08 \times Van^1(C_n) + 2.28$	$R = 0.4288$	$R^2 = 0.1839$
RT1	$RT1 = 0.0039 \times Van^1(C_n) + 0.782$	$R = 0.058$	$R^2 = 0.0034$
RT2	$RT2 = 0.0627 \times Van^1(C_n) + 2.169$	$R = 0.3135$	$R^2 = 0.0983$
SR1	$SR1 = 0.0002 \times Van^1(C_n) + 0.0649$	$R = 0.0293$	$R^2 = 0.0009$
SR2	$SR2 = 0.0004 \times Van^1(C_n) + 1.0859$	$R = 0.0052$	$R^2 = 0$
HoF	$HoF = 36.2455 \times Van^1(C_n) + 401.037$	$R = 0.9444$	$R^2 = 0.8919$

4. Conclusions

In this study, Van molecular topological indices that are associated with the physical characteristics of fullerene are calculated. Fullerene balls C₅₄, C₅₈, C₆₀, C₇₀, C₇₄, C₇₈, C₈₀, C₈₂, C₈₄, C₈₆, and C₉₀ are taken into account. The chemical structures are mapped and displayed graphically. The degree of each vertex of the chemical graph was found to be three. A regression line is fitted to the data before linear regression analysis. The most accurate representation of the data is a regression line, which uses the well-known least squares fit. For the data, we estimated the correlation coefficient and the coefficient of determination. According to the regression analysis of six Van indices dependent on each other, all the indices for these structures are highly related to the first Van index. We considered the fullerene "cages" physical characteristics, such as RT-1, BEs, RT-2, SR-1, Hof, and SR-2. These attributes are subjected to a linear regression analysis based on the first Van index. Physical characteristics such as the second and first Ramsauer-Townsend minima, binding energies, and the second and first shape had a strong correlation with the first Van index. However, the first Van index, of which the coefficient of determination is high and an elevated correlation coefficient, best captures the heat of structure creation. Therefore, we can conclude that the first Van index, which has a substantial influence on it, is the best to forecast the heat of formation of fullerene structures. Notably, this study focuses on predicting fullerene physical features using the first Van index. It is discovered that the developed linear regression relation may predict the heat of formation with the best degree of accuracy. Systematizing biochemical, medicinal, and ecological knowledge pertinent to utilizing fullerenes may be accomplished using these models. This systematization steadily acquires a major role as the number of fullerene applications increases daily.

Author Contributions

All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement

Data supporting the findings of this study are available upon reasonable request from the corresponding author.

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Conflicts of Interest

The authors declare no conflict of interest.

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