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Exploring Topological Indices and Power Curve Fitting Models for Predicting Heat of Formation in Magnesium Aluminate Network

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Abstract

The prediction of thermodynamic properties using mathematical and graph-theoretical approaches has secured significant attention in materials science. The current paper is a statistical investigation of the relationship between various topological indices and the heat of formation (HOF) of the Magnesium aluminate $MgAl_2O_4$ network. The study fills the current gap in the systematic relationship between graph-theoretical descriptors and thermodynamic stability of structured $MgAl_2O_4$ networks. The HOF data is computed using a computational simulation of the related network structures under homogeneous reference conditions whereby consistency is applied in the energy assessment mechanism. Moreover the present study show a statistical insight into how different topological indices express the heat of formation in the Magnesium aluminate ($MgAl_2O_4$) network. By taking into account various topological indices, we use a power curve-fitting technique to speculate and describe the heat of formation-an major thermodynamic element that directly act on the stability and reactivity of ($MgAl_2O_4$). We compute and investigate the Randic index, the Atom-Bond Connectivity (ABC) index, the Geometric-Arithmetic (GA) index, and the Zagreb index based on the chemical graph depiction in case of the HOF data. Results indicate significant predictive efficiency, with the value of R_1 having the best fit ($R^2 = 0.9998$, $RMSE = 4.525610^{-23}$), followed by R_{-1} and GA indices. All other indices have shown to have strong correlations ($R^2 > 0.96$). It is thus evident that power fitting helps in estimating the value of HOF effectively and successfully. We also found some important connections among heat of formation and topological indicators applying the power curve-fitting method. Our outcome gives proof that the curve-fitted model not only provides accurate results of the data points but also assists a good perception of the nature of the chemical interlinking within the ($MgAl_2O_4$) network.

Keywords: Magnesium Aluminate $MgAl_2O_4$; Topological indices; Randic indices; ABC indices; Multiple Zagreb indices Statistical analysis; heat of formation; Power curve fitting method .

1 Introduction

In graph theory, a graph is a mathematical appliance that shows how different things link together. A graph consists of nodes and edges. The point is called nodes or vertices, and the connection between these points is called links or edges. Usually, nodes and edges are considered by V and E individually. Generally, a graph is represented by $G = (V, E)$. Molecular graph theory is a particular side of graph theory. In which we work on the modeling and structures of Molecules through graphs. In this case, the chemical bonds between atoms show the edges(links) and the atoms are nodes(vertices). Its useful to deal with the structure, characteristics and relation of Molecules and is significant in different fields e.g biology and chemistry etc. Using data about how atoms are connected, chemical graph theory can guess the structures of Molecules [1]. The strength of links(edges) that connect a node(vertex) μ in graph G is called the degree of that vertex, $\psi(\mu)$.

Firstly, the idea of topological indices given by Harold Wiener in 1947. Wiener approximate the boiling point of paraffin using these indices. [2, 3]. A numerical value of a molecular structure that rely on the connectivity of that structure is said to be a topological index [4]. Topological indices relating molecular structure with there chemical and physical characteristics, in chemical graph theory studies [5]. Prediction of many characteristics of chemical compound like enthalpy of formation, entropy, melting and boiling points with help of topological indices, excluding the laboratory experiments [6]. The bibliometric graph present that the main research idea in the arae of topological indices based on algebraic graph theory, chemical structural theory, and nanomaterial. The key terms related to this research are "Randic indices," "Hyper Zagreb indices," and "branch graphs," presenting their significance in graphical and quantitative analysis [7, 8].

The degree-based topological co-indices make an important family of molecular descriptors in chemical graph theory as they rely on the degree of a vertex in a molecular structure, which represents an atom [12]. Unlike the typical degree based topological indices, co-indices are computed using pairs of non adjacent vertebrae, thereby giving complementary data on the molecular graph. The most prominent ones are the former and the latter Zagreb co-index, the harmonic co-index, and the atom–bond connectivity (ABC) co-index [13]. In quantitative structure-property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies, these indices are widely employed to model and predict multiple physicochemical properties, such as heat of formation, boiling point, enthalpy, stability and biological activity of chemical compounds [14]. It has been demonstrated in the past studies that co-indices of degree can be used to differentiate between molecular structures that have similar connectivity and can be effectively applied on nanostructures, metal-organic networks and complex inorganic networks [15]. They have also found application in materials science, where they are used to correlate structural properties with the thermodynamic properties and offer valuable information about the design and optimization of compounds like magnesium aluminate networks [16].



Magnesium aluminate, $MgAl_2O_4$, is a strong ceramic with a cubic spinel crystal structure. In this lattice, magnesium ions (Mg^{+2}) engage tetrahedral shape while aluminum ions (Al^{+3}) are found in octahedral shape within a dense-packed network of oxygen ions. With this specific kind of order within $MgAl_2O_4$, it follows that the material is very stable opposed to heat and chemicals, unbreakable, and has wide energy gap. Due to these characters, $MgAl_2O_4$ is generally used in very high-temperature circumstances, for instance, the inner walls of furnaces and kilns. [17]. In

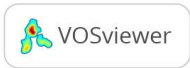


Figure 2: The Bibliometric Analysis of Topological Indices

the current study we calculated the various topological indices of the chemical structure of magnesium aluminate, $MgAl_2O_4$, and investigate the comprehensive inter-relations between the heat of formation of the $MgAl_2O_4$ network with the topological indices. The structure of molecules or crystals is presented by topological indices that depend on the connected atoms. In the case of magnesium aluminate, $MgAl_2O_4$, topological indices describe how difference in the order of Mg , Al , and O atoms result in the stability of the material. A scientific study of its variation with various topological indices is thus essential to understand their relation. An suitable power curve model of the form $y = ax^b + c$ was used; here, x is the topological index and y is the heat of formation. Such a model show almost all the characteristics of inorganic materials, variation nonlinearly with their structure. Applying such a model useful to explaining the energy stability due to variation in the structure for better conception of how the atomic arrangement impact the heat of formation of $MgAl_2O_4$. [20].

In the earlier studies, the thermodynamic property and stability of magnesium aluminate and related oxide materials have been examined only through experimental methods without predictive method. For example, the enthalpies of solution were normally calculated using high-temperature oxide melt solution calorimetry, which gives exact thermodynamic data but require complicated laboratory apparatus [22]. In the present study, the heat of formation was measured through experiments without using any modeling technique or analytical optimization techniques [23]. Most of the material characterizations made in these studies take part bulk testing and macroscopic quantifying and not inspection on molecular level insights [23]. Also, molecular structure was considered an insignificant factor for the characterization of the materials; so, the fundamental connection existing between the structure and characteristics was not fully realized [24]. The thermodynamic parameters were generally calculated only after the fusion of the material; this indicate an empirical way rather than estimated or simulation-based methods [24]. Also, predictive structural modeling mechanism was not work in these studies, and because of that, the thermodynamic characteristics estimated using known structural properties was also finite [25]. These deficiency specify the essential for advance analytical methods using which a more perfect and expected understanding of the heat of formation and stability of $MgAl_2O_4$ and other spinel-type materials is advanced using molecular topology, computational modeling and thermodynamic link techniques. The alliance of this study with earlier research on Magnesium aluminate and related systems is shown in Table 1.

The Vertex-degree-based indices, which are based on the graph's node degree, are a specific type of topological index.[26, 27]. The General Randic index [28]is a method that chemical engineers use to its properties.

Table 1: Aspects, Novel Contributions, and Gaps Addressed in This Work

Aspect	This Work	Novel Contribution	Gap Addressed
Structural representation	Graph based representation of $MgAl_2O_4$ network	Uses chemical graph modeling for structural analysis	Enables graph theoretic descriptors linking local and global structure [21]
Topological indices used	Advanced degree-based indices and co-indices	Incorporates multiple indices capturing complex topology	Captures multi-scale topology and spinel-specific features [22]
Modeling approach	Regression-based curve fitting models	Hybrid mathematical and statistical modeling	Improves predictive accuracy and reduces overfitting [23]
Data sources and curation	Carefully constructed dataset from computed indices	Standardized and reproducible data preparation	Provides robust, reproducible dataset with quality assurance [23]
Validation strategy	Model validation using statistical measures	Comparative evaluation of model performance	Demonstrates generalizability and stability of models [24]
Thermodynamic prediction	Prediction of heat of formation (HOF)	Direct linkage between structure and thermodynamic property	Bridges gap between topology and thermodynamics [24]
Application scope	Focus on magnesium aluminate network	Extends applicability to inorganic networks	Expands use of topological indices in materials science [25]

$R_\alpha(G)$ are introduced by Amic et al. [29] and Bollobás et al. [30] as:

$$R_\alpha(G) = \sum_{\mu\nu \in E(G)} (\mathfrak{Z}(\mu) \times \mathfrak{Z}(\nu))^\alpha, \text{ Where } \alpha = 1, -1, \frac{1}{2}, -\frac{1}{2} \quad (1)$$

The $ABC(G)$ indices generated by Estrada et al. [34, 35] these indices give us bio-activity and chemico-physical aspect [31, 32, 33].

$$ABC(G) = \sum_{\mu\nu \in E(G)} \sqrt{\frac{\mathfrak{Z}(\mu) + \mathfrak{Z}(\nu) - 2}{\mathfrak{Z}(\mu) \times \mathfrak{Z}(\nu)}}. \quad (2)$$

Vukicevic et al. [36] computed the GA indices as:

$$GA(G) = \sum_{\mu\nu \in E(G)} \frac{2\sqrt{\mathfrak{Z}(\mu) \times \mathfrak{Z}(\nu)}}{\mathfrak{Z}(\mu) + \mathfrak{Z}(\nu)}. \quad (3)$$

$M_1(G)$ and $M_2(G)$ presented [37, 38] by Gutman as:

$$M_1(G) = \sum_{\mu\nu \in E(G)} (\mathfrak{Z}(\mu) + \mathfrak{Z}(\nu)). \quad (4)$$

$$M_2(G) = \sum_{\mu\nu \in E(G)} (\mathfrak{Z}(\mu) \times \mathfrak{Z}(\nu)). \quad (5)$$

$HM(G)$ determined by [39] Shirdal et al. that presented in this way:

$$HM(G) = \sum_{\mu\nu \in E(G)} (\mathfrak{Z}(\mu) + \mathfrak{Z}(\nu))^2. \quad (6)$$

Ghorbani and Azimi described $PM_1(G)$ and $PM_2(G)$ [40], shown as:

$$PM_1(G) = \prod_{\mu\nu \in E(G)} (\mathfrak{Z}(\mu) + \mathfrak{Z}(\nu)). \quad (7)$$

$$PM_2(G) = \prod_{\mu\nu \in E(G)} (\mathfrak{Z}(\mu) \times \mathfrak{Z}(\nu)). \quad (8)$$

$ReZG_1(G)$, $ReZG_2(G)$ and $ReZG_3(G)$ indices computed by Rajini [41] in this way:

$$ReZG_1(G) = \sum_{\mu\nu \in E(G)} \frac{\mathfrak{Z}(\mu) + \mathfrak{Z}(\nu)}{\mathfrak{Z}(\mu) \times \mathfrak{Z}(\nu)}. \quad (9)$$

$$ReZG_2(G) = \sum_{\mu\nu \in E(G)} \frac{\mathfrak{Z}(\mu) \times \mathfrak{Z}(\nu)}{\mathfrak{Z}(\mu) + \mathfrak{Z}(\nu)}. \quad (10)$$

$$ReZG_3(G) = \sum_{\mu\nu \in E(G)} (\mathfrak{Z}(\mu) \times \mathfrak{Z}(\nu))(\mathfrak{Z}(\mu) + \mathfrak{Z}(\nu)). \quad (11)$$

The developing advances in the field of chemical graph theory maintain the great role that topological indices use to estimate the molecular behavior and characteristics. ABC, Randic, and Zagreb indices are work to investigate the nano structure and their thermodynamic property like heat of formation are presented in past [42, 43].

2 Structure of Magnesium aluminate ($MgAl_2O_4$)

Magnesium aluminate ($MgAl_2O_4$) [42] has a spinel crystal structure, which is a type of arrangement where oxide ions (O^{2-}) are packed closely in a cubic pattern. Magnesium (Mg^{2+}) and aluminum (Al^{3+}) ions are placed in specific positions within this structure. The oxide ions form a face-centered cubic (FCC) lattice, and magnesium ions take up one-eighth of the tetrahedral sites, while aluminum ions occupy half of the octahedral sites. This organized arrangement makes magnesium aluminate very stable and hard. The spinel structure is symmetrical and tightly packed, which gives the material good thermal stability, strength, and resistance to chemical reactions. Because of these qualities, magnesium aluminate is commonly used in ceramics, high-temperature materials, and as a base material in electronics. The Molecular structure of Magnesium Aluminate ($MgAl_2O_4$) for $[m, n] = [1, 1]$, $[m, n] = [1, 2]$ are shown by Figure 3.

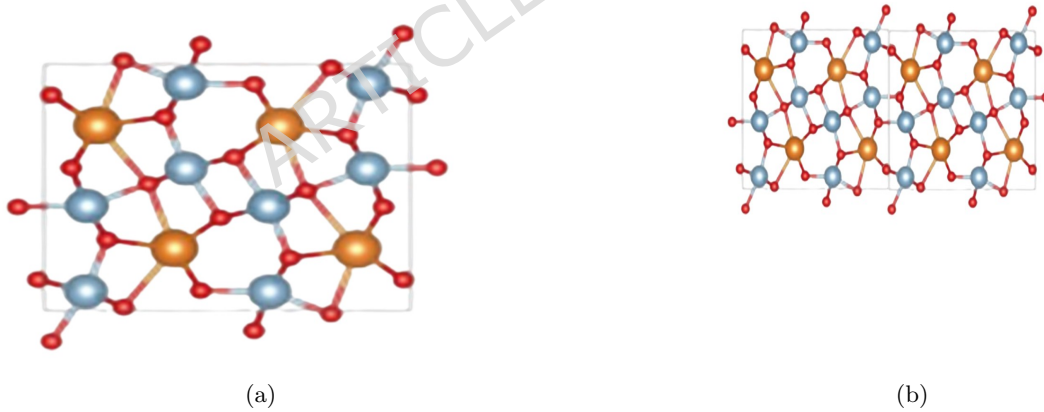


Figure 3: (a)The structure of Magnesium aluminate ($MgAl_2O_4$) for $[m, n] = [1, 1]$; (b)The structure of Magnesium aluminate ($MgAl_2O_4$) for $[m, n] = [1, 2]$ [42]

The order of ($MgAl_2O_4$) is $28mn + 6m + 4n$. And $52mn$ is the length or size of $MgAl_2O_4$. Table 2 present the vertex partition. Table 3 describe the edge partition.

$\mathfrak{Z}(\mu)$	Frequency	Set of vertices
1	$4m + 4n + 2$	V_1
2	$8m + 4n - 4$	V_2
3	$12mn - 4m - 4n + 2$	V_3
4	$12mn - 2m$	V_4
5	$4mn$	V_5

Table 2: Vertex Partition of ($MgAl_2O_4$).

$(\beth(\mu), \beth(\nu))$	Frequency	Set of edges
(1,4)	$4m + 4n$	E_1
(1,5)	2	E_2
(2,4)	$8m + 4n - 4$	E_3
(2,5)	$8m + 4n - 4$	E_4
(3,4)	$24mn - 8m - 8n + 4$	E_5
(3,5)	$12mn - 4m - 4n + 2$	E_6
(4,4)	$8mn - 4m$	E_7
(4,5)	$8mn - 4m$	E_8

Table 3: Edge Partition of $(MgAl_2O_4)$.

3 Indices computation for Magnesium Aluminate $(MgAl_2O_4)$

- The Randic Index

$$R_\alpha(G) = \sum_{\mu\nu \in E(MgAl_2O_4)} (\beth(\mu) \times \beth(\nu))^\alpha; \quad \alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}$$

For $\alpha = 1$;

$$\begin{aligned}
R_1(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} (\beth(\mu) \times \beth(\nu))^1 \\
&= (1 \times 4)(4m + 4n) + (1 \times 5)2 + (2 \times 4)(8m + 4n - 4) \\
&+ (2 \times 5)(8m + 4n - 4)(3 \times 4)(24mn - 8m - 8n + 4) \\
&+ (3 \times 5)(12mn - 4m - 4n + 2)(4 \times 4)(8mn - 4m) \\
&+ (4 \times 5)(8mn - 4m). \\
&= 756mn - 140m - 68n + 16.
\end{aligned}$$

For $\alpha = -1$;

$$\begin{aligned}
R_{-1}(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} (\beth(\mu) \times \beth(\nu))^{-1} \\
&= \frac{1}{1 \times 4}(4m + 4n) + \frac{1}{1 \times 5}2 + \frac{1}{2 \times 4}(8m + 4n - 4) \\
&+ \frac{1}{2 \times 5}(8m + 4n - 4)\frac{1}{3 \times 4}(24mn - 8m - 8n + 4) \\
&+ \frac{1}{3 \times 5}(12mn - 4m - 4n + 2) + \frac{1}{4 \times 4}(8mn - 4m) \\
&+ \frac{1}{4 \times 5}(8mn - 4m) \\
R_{-1}(MgAl_2O_4) &= \frac{37}{10}mn + \frac{17}{12}m + \frac{29}{30}n - \frac{1}{30}
\end{aligned}$$

For $\alpha = \frac{1}{2}$;

$$\begin{aligned}
 R_{\frac{1}{2}}(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} (\beth(\mu) \times \beth(\nu))^{\frac{1}{2}} \\
 &= \sqrt{(1 \times 4)(4m + 4n)} + \sqrt{(1 \times 5)2} + \sqrt{(2 \times 4)(8m + 4n - 4)} \\
 &+ \sqrt{(2 \times 5)(8m + 4n - 4)}\sqrt{(3 \times 4)(24mn - 8m - 8n + 4)} \\
 &+ \sqrt{(3 \times 5)(12mn - 4m - 4n + 2)} + \sqrt{(4 \times 4)(8mn - 4m)} \\
 &+ \sqrt{(4 \times 5)(8mn - 4m)}. \\
 &= 197.388mn - 21.172m - 11.244n - 7.866.
 \end{aligned}$$

For $\alpha = -\frac{1}{2}$;

$$\begin{aligned}
 R_{-\frac{1}{2}}(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} \frac{1}{\sqrt{(\beth(\mu) \times \beth(\nu))}} \\
 &= \frac{1}{\sqrt{1 \times 4}}(4m + 4n) + \frac{1}{\sqrt{1 \times 5}}2 + \frac{1}{\sqrt{2 \times 4}}(8m + 4n - 4) \\
 &+ \frac{1}{\sqrt{2 \times 5}}(8m + 4n - 4)\frac{1}{\sqrt{3 \times 4}}(24mn - 8m - 8n + 4) \\
 &+ \frac{1}{\sqrt{3 \times 5}}(12mn - 4m - 4n + 2)\frac{1}{\sqrt{4 \times 4}}(8mn - 4m) \\
 &+ \frac{1}{\sqrt{4 \times 5}}(8mn - 4m) \\
 &= 13.8154mn + 2.1216m + 1.3369n - 0.1136.
 \end{aligned}$$

Numerical investigation and visually representation of $R_\alpha(MgAl_2O_4)$ given in Table 4 and Figure 4.

$[m, n]$	$R_1(MgAl_2O_4)$	$R_{-1}(MgAl_2O_4)$	$R_{\frac{1}{2}}(MgAl_2O_4)$	$R_{-\frac{1}{2}}(MgAl_2O_4)$
[1, 1]	564	6.05	157.106	17.1603
[2, 2]	2624	19.53	716.854	62.0650
[3, 3]	6196	40.42	1671.378	134.6005
[4, 4]	11280	68.70	3020.678	234.7668
[5, 5]	17876	104.38	4764.754	362.5639
[6, 6]	25984	147.47	6903.606	517.9918
[7, 7]	35604	197.95	9437.234	701.0505
[8, 8]	46736	255.8333	12365.638	911.7400
[9, 9]	59380	321.1167	15688.818	1150.0603
[10, 10]	73536	393.8000	19406.774	1416.0114

Table 4: Quantitative analysis of $R_1(MgAl_2O_4)$, $R_{-1}(MgAl_2O_4)$, $R_{\frac{1}{2}}(MgAl_2O_4)$, and $R_{-\frac{1}{2}}(MgAl_2O_4)$.

Table 4 displays the numerical study of several topological indices for varying values of $[m, n]$. These are: $R_1(MgAl_2O_4)$, $R_{-1}(MgAl_2O_4)$, $R_{\frac{1}{2}}(MgAl_2O_4)$ and $R_{-\frac{1}{2}}(MgAl_2O_4)$. These indices show the chemical structure and characteristics of the $(MgAl_2O_4)$ network. The analysis of the Randic indices for $MgAl_2O_4$ shows that all the index values consistently increase as the molecular parameters $[m, n]$ change. Out of the four indices, $R_1(MgAl_2O_4)$ and $R_{\frac{1}{2}}(MgAl_2O_4)$ grow quickly and in a non-linear way, which means they are very sensitive to how big and complex the molecule is. On the other hand, $R_{-1}(MgAl_2O_4)$ and $R_{-\frac{1}{2}}(MgAl_2O_4)$ increase more slowly, almost in a straight line. Looking at the statistical results, $R_1(MgAl_2O_4)$ has the highest average and the biggest spread, showing a lot of variation in the data. Meanwhile, $R_{-1}(MgAl_2O_4)$ has the smallest values and the least variation. The steady increase in all the indices suggests that the way the molecule is structured has a direct effect on how connected it is. In general, the results show that as the molecule contains larger, the Randic indices specifically those with positive exponents change more observable, express a strong connection among the structure and its connectivity.

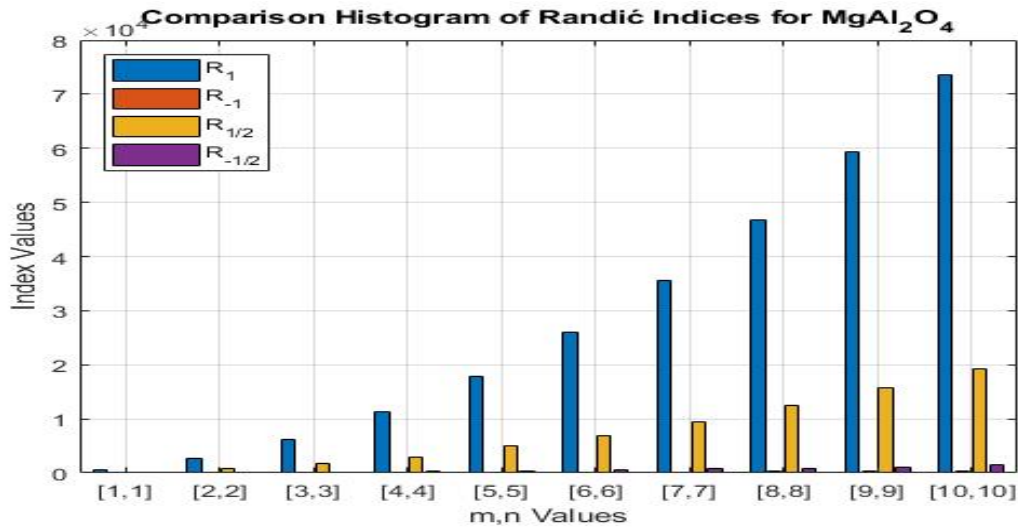


Figure 4: Graphical depiction $R_1(MgAl_2O_4)$, $R_{-1}(MgAl_2O_4)$, $R_{\frac{1}{2}}(MgAl_2O_4)$ and $R_{-\frac{1}{2}}(MgAl_2O_4)$

Figure 4 The histogram shows how the Randić type topological indices R_1 , R_{-1} , $R_{\frac{1}{2}}$, and $R_{-\frac{1}{2}}$ behave as the values of (m, n) increase for the structure of $MgAl_2O_4$. From the graph, it's clear that all four indices increase steadily, which happens because the graph becomes larger and more complex as $[m, n]$ grows. However, the way each index increases is different. Among the four, $R_{\frac{1}{2}}$ has the highest values and grows the fastest. This suggests that this index is very responsive to changes in the graph's size and how degrees are distributed across vertices. The index $R_{-\frac{1}{2}}$ also rises with $[m, n]$, but it stays much lower, showing a moderate sensitivity to vertex degrees. On the other hand, R_1 increases in a steady and consistent way. Meanwhile, R_{-1} has the smallest values and grows the slowest, which is because it is inversely related to the degrees of the vertices.

• Atom Bond Connectivity Index

$$\begin{aligned}
 ABC(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} \sqrt{\frac{(\mathfrak{D}(\mu) + \mathfrak{D}(\nu) - 2)}{\mathfrak{D}(\mu) \times \mathfrak{D}(\nu)}} \\
 ABC(MgAl_2O_4) &= \sqrt{\frac{1+4-2}{(1 \times 4)}}(4m+4) + \sqrt{\frac{1+5-2}{(1 \times 5)}}(2) \\
 &+ \sqrt{\frac{2+4-2}{(2 \times 4)}}(8m+4n-4) + \sqrt{\frac{2+5-2}{(2 \times 5)}}(8m+4n-4) \\
 &+ \sqrt{\frac{3+4-2}{(3 \times 4)}}(24mn-8m-8n+4) \\
 &+ \sqrt{\frac{3+5-2}{(3 \times 5)}}(12mn-4m-4n+2) \\
 &+ \sqrt{\frac{4+4-2}{(4 \times 4)}}(8mn-4m) + \sqrt{\frac{4+5-2}{(4 \times 5)}}(8mn-4m) \\
 &= 32.714mn + 2.270m + 1.427n - 0.020.
 \end{aligned}$$

• Geometric Arithmetic Index

$$\begin{aligned}
GA(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} \frac{2\sqrt{\beth(\mu) \times \beth(\nu)}}{\beth(\mu) + \beth(\nu)} \\
&= \frac{2\sqrt{1 \times 4}}{(1+4)}(4m+4n) + \frac{2\sqrt{1 \times 5}}{(1+5)}(2) \\
&+ \frac{2\sqrt{2 \times 4}}{(2+4)}(8m+4n-4) + \frac{2\sqrt{2 \times 5}}{(2+5)}(8m+4n-4) \\
&+ \frac{2\sqrt{3 \times 4}}{(3+4)}(24mn-8m-8n+4) + \frac{2\sqrt{3 \times 5}}{(3+5)}(12mn-4m-4n+2) \\
&+ \frac{2\sqrt{4 \times 4}}{(4+4)}(8mn-4m) + \frac{2\sqrt{4 \times 5}}{(4+5)}(8mn-4m) \\
&= 51.323mn - 1.796m - 1.206n + 0.001.
\end{aligned}$$

• The First Zagreb Index

$$\begin{aligned}
M_1(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} (\beth(\mu) + \beth(\nu)) \\
&= (1+4)(4m+4n) + (1+5)(2) + (2+4)(8m+4n-4) \\
&+ (2+5)(8m+4n-4) + (3+4)(24mn-8m-8n+4) \\
&+ (3+5)(12mn-4m-4n+2) \\
&+ (4+4)(8mn-4m) + (4+5)(8mn-4m) \\
&= 400mn - 32m - 16n + 4.
\end{aligned}$$

• The Second Zagreb Index

$$\begin{aligned}
M_2(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} (\beth(\mu) \times \beth(\nu)) \\
&= (1 \times 4)(4m+4n) + (1 \times 5)(2) + (2 \times 4)(8m+4n-4) \\
&+ (2 \times 5)(8m+4n-4) + (3 \times 4)(24mn-8m-8n+4) \\
&+ (3 \times 5)(12mn-4m-4n+2) + (4 \times 4)(8mn-4m) \\
&+ (4 \times 5)(8mn-4m) \\
&= 756mn - 140m - 68n + 16.
\end{aligned}$$

Numerical investigation and visually representation of $ABC(MgAl_2O_4)$, $GA(MgAl_2O_4)$, $M_1(MgAl_2O_4)$, and $M_2(MgAl_2O_4)$ given in Table 5 and Figure 5 individually.

Table 5 show the quantitative study of various chemical descriptors and topological index for the $(MgAl_2O_4)$ depending on the values of $[m, n]$. The quantitative analysis of $AB(MgAl_2O_4)$, $GA(MgAl_2O_4)$, $M_1(MgAl_2O_4)$, and $M_2(MgAl_2O_4)$ shows a steady increase as the values of m and n go from 1 to 10. These four index raise significantly with this variation, presenting a direct connection with the multiplication of m and n . Such as, $ABC(MgAl_2O_4)$ growing from 36.391 to 3308.350, and $GA(MgAl_2O_4)$ raises from 48.322 to 5102.281. In parallel, $GA(MgAl_2O_4)$ and $M_1(MgAl_2O_4)$ boost up from 356 to 39524 and from 564 to 73536, separately. This regular form show that the structural and topological properties of $MgAl_2O_4$ are very receptive to vary in m and n , describe a hard positive link among these variables. The results confirm that as molecular complexity or degree parameters increase, the topological descriptors also increase significantly.

$[m, n]$	$ABC(MgAl_2O_4)$	$GA(MgAl_2O_4)$	$M_1(MgAl_2O_4)$	$M_2(MgAl_2O_4)$
[1, 1]	36.391	48.322	356	564
[2, 2]	138.230	199.289	1508	2496
[3, 3]	305.497	452.902	3460	5904
[4, 4]	538.192	809.161	6212	10888
[5, 5]	836.315	1268.066	9764	17648
[6, 6]	1199.866	1829.617	14116	26284
[7, 7]	1628.845	2493.814	19268	36796
[8, 8]	2123.252	3260.657	25220	46736
[9, 9]	2683.087	4130.146	31972	59380
[10, 10]	3308.350	5102.281	39524	73536

Table 5: Numeric study $ABC(MgAl_2O_4)$, $GA(MgAl_2O_4)$, $M_1(MgAl_2O_4)$ and $M_2(MgAl_2O_4)$.

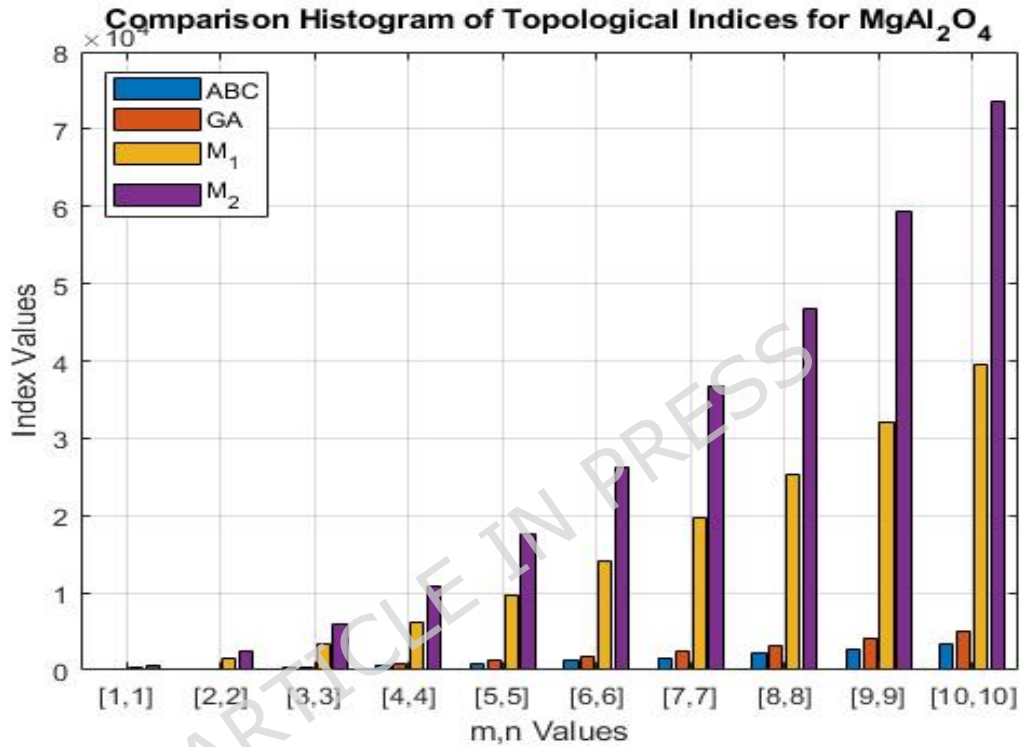


Figure 5: Graphical depiction $ABC(MgAl_2O_4)$, $GA(MgAl_2O_4)$, $M_1(MgAl_2O_4)$ and $M_2(MgAl_2O_4)$

The relation between topological indices of ABC, GA, M_1 and M_2 of the Magnesium Aluminate ($MgAl_2O_4$) are presented in Figure 5. The histogram shows how the four topological indices $ABC(MgAl_2O_4)$, $GA(MgAl_2O_4)$, $M_1(MgAl_2O_4)$, and $M_2(MgAl_2O_4)$ change with respect to the parameters m and n . From the graph, it's clear that all four indices increase consistently as the values of m and n go from 1 to 10. Among them, $M_2(MgAl_2O_4)$ increases the most, followed by $M_1(MgAl_2O_4)$, showing that these indices are highly sensitive to changes in the parameters. On the other hand, $ABC(MgAl_2O_4)$ and $GA(MgAl_2O_4)$ increase more slowly. The overall pattern shows that as m and n get larger, the topological indices also rise, which means the molecular structure becomes more complex with increasing values of these parameters.

- Hyper Zagreb Index

$$\begin{aligned}
HM(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} (\beth(\mu) + \beth(\nu))^2 \\
&= (1+4)^2(4m+4n) + (1+5)^2(2) + (2+4)^2(8m+4n-4) \\
&+ (2+5)^2(8m+4n-4) + (3+4)^2(24mn-8m-8n+4) \\
&+ (3+5)^2(12mn-4m-4n+2) + (4+4)^2(8mn-4m) \\
&+ (4+5)^2(8mn-4m) \\
&= 3104mn - 448m - 208n + 56.
\end{aligned}$$

• **First Multiple Zagreb Index**

$$\begin{aligned}
PM_1(MgAl_2O_4) &= \prod_{i=1}^8 \prod_{\mu\nu \in E_i(MgAl_2O_4)} (\beth(\mu) + \beth(\nu)) \\
&= ((1+4) \times (4m+4n)) \times ((1+5) \times (2)) \times ((2+4) \times (8m+4n-4)) \\
&\times ((2+5) \times (8m+4n-4)) \times ((3+4) \times (24mn-8m-8n+4)) \\
&\times ((3+5) \times (12mn-4m-4n+2)) \times ((4+4) \times (8mn-4m)) \\
&\times ((4+5) \times (8mn-4m)) \\
&= 83235962880m^2(m+n)(2n-1)^2(2m+n-1)^2(6mn-2m-2n+1)^2
\end{aligned}$$

• **Second Multiple Zagreb Index**

$$\begin{aligned}
PM_2(MgAl_2O_4) &= \prod_{i=1}^8 \prod_{\mu\nu \in E_i(MgAl_2O_4)} (\beth(\mu) \times \beth(\nu)) \\
&= (1 \times 4) \times (4m+4n) \times (1 \times 5) \times (2) \times (2 \times 4) \times (8m+4n-4) \\
&\times (2 \times 5) \times (8m+4n-4) \times (2 \times 5) \times (8m+4n-4) \times (3 \times 4) \\
&\times (24mn-8m-8n+4) \\
&\times (3 \times 5) \times (12mn-4m-4n+2) \\
&\times (4 \times 4) \times (8mn-4m) \times (4 \times 5) \times (8mn-4m) \\
&= 755220480000(m+n)(2m+n-1)^3 \\
&\times (24mn-8m-8n+4)(12mn-4m-2)m^2(2n-1)^2
\end{aligned}$$

Numerical investigation and visually representation of $HM(MgAl_2O_4)$, $PM_1(MgAl_2O_4)$ and $PM_2(MgAl_2O_4)$ given in Table 6 and Figure 6 individually.

$[m, n]$	$HM(MgAl_2O_4)$	$PM_1(MgAl_2O_4)$	$PM_2(MgAl_2O_4)$
[1, 1]	2504	5.993×10^{12}	8.7001×10^{15}
[2, 2]	11160	4.334×10^{16}	3.5126×10^{20}
[3, 3]	26024	4.434×10^{19}	8.4398×10^{22}
[4, 4]	47096	1.039×10^{20}	3.5542×10^{24}
[5, 5]	74400	9.69×10^{20}	6.1130×10^{25}
[6, 6]	107864	6.30×10^{21}	6.0790×10^{26}
[7, 7]	147560	3.12×10^{22}	4.1742×10^{27}
[8, 8]	193464	1.26×10^{24}	2.19×10^{28}
[9, 9]	245576	4.82×10^{24}	9.42×10^{28}
[10, 10]	303896	1.59×10^{25}	3.45×10^{29}

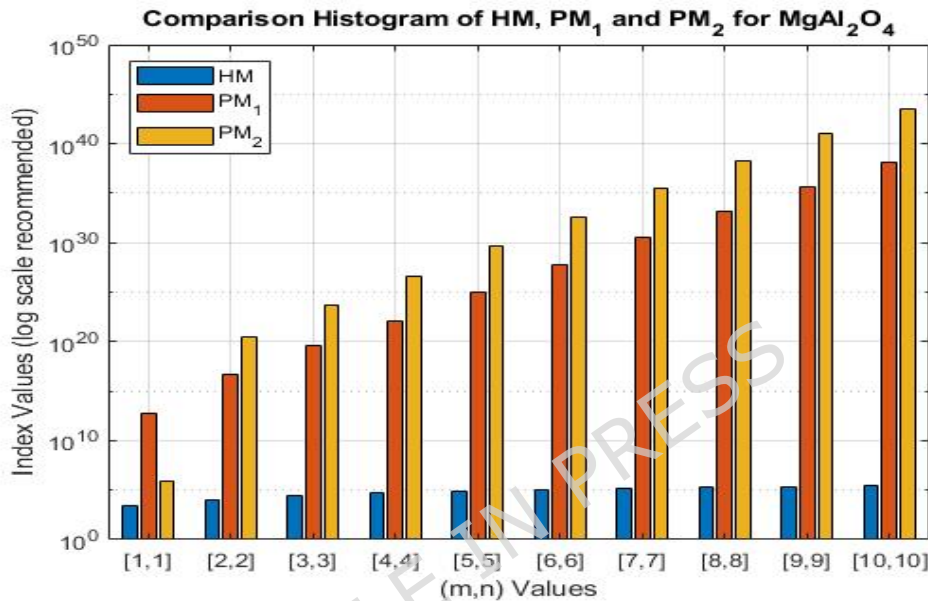
Table 6: Quantitative analysis $HM(MgAl_2O_4), PM_1(MgAl_2O_4), PM_2(MgAl_2O_4)$ Figure 6: Graphical depiction $HM(MgAl_2O_4), PM_1(MgAl_2O_4)$ and $PM_2(MgAl_2O_4)$

Figure 6 show the comparative growing at a constant proportional rate in the HM , PM_1 and PM_2 of the Magnesium Aluminate ($MgAl_2O_4$) network. The outcome show that all three variables increase in manner as m and n going larger, presenting a good connection among the size of the structure and the values of these molecular indices. Generally, the harmonic mean index $HM(MgAl_2O_4)$ growing slowly from 2504 at [1, 1] to 303896 at [10, 10]. Instead, $PM_1(MgAl_2O_4)$ and $PM_2(MgAl_2O_4)$ raise exponentially, gain the values of 1.59×10^{25} and 3.45×10^{29} , individually. This high rate growth show that these product-based indices are very receptive to variation in size and have strong potential for guess molecular complexity and topological characteristics of $MgAl_2O_4$ structures.

• Redefined First Zagreb Index

$$\begin{aligned}
 ReZG_1(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} \frac{\mathfrak{Z}(\mu) + \mathfrak{Z}(\nu)}{\mathfrak{Z}(\mu) \times \mathfrak{Z}(\nu)} \\
 &= \left(\frac{1+4}{1 \times 4} \right) (4m + 4n) + \left(\frac{1+5}{1 \times 5} \right) (2) + \left(\frac{2+4}{2 \times 4} \right) (8m + 4n - 4) \\
 &+ \left(\frac{2+5}{2 \times 5} \right) (8m + 4n - 4) + \left(\frac{3+4}{3 \times 4} \right) (24mn - 8m - 8n + 4) \\
 &+ \left(\frac{3+5}{3 \times 5} \right) (12mn - 4m - 4n + 2) \\
 &+ \left(\frac{4+4}{4 \times 4} \right) (8mn - 4m) + \left(\frac{4+5}{4 \times 5} \right) (8mn - 4m) \\
 &= 28mn + 6m + 4n.
 \end{aligned}$$

• **Redefined Second Zagreb Index**

$$\begin{aligned}
ReZG_2(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} \frac{\beth(\mu) \times \beth(\nu)}{\beth(\mu) + \beth(\nu)} \\
&= \left(\frac{1 \times 4}{1+4} \right) (4m + 4n) + \left(\frac{1 \times 5}{1+5} \right) (2) + \left(\frac{2 \times 4}{2+4} \right) (8m + 4n - 4) \\
&+ \left(\frac{2 \times 5}{2+5} \right) (8m + 4n - 4) + \left(\frac{3 \times 4}{3+4} \right) (24mn - 8m - 8n + 4) \\
&+ \left(\frac{3 \times 5}{3+5} \right) (12mn - 4m - 4n + 2) + \left(\frac{4 \times 4}{4+4} \right) (8mn - 4m) \\
&+ \left(\frac{4 \times 5}{4+5} \right) (8mn - 4m) \\
&= 97.42mn - 12.81m - 6.97n + 1.23
\end{aligned}$$

• **Redefined Third Zagreb Index**

$$\begin{aligned}
ReZG_3(MgAl_2O_4) &= \sum_{i=1}^8 \sum_{\mu\nu \in E_i(MgAl_2O_4)} (\beth(\mu) \times \beth(\nu)) (\beth(\mu) + \beth(\nu)) \\
&= (1 \times 4)(1+4)(4m + 4n) + (1 \times 5)(1+5)(2) \\
&+ (2 \times 4)(2+4)(8m + 4n - 4) + (2 \times 5)(2+5)(8m + 4n - 4) \\
&+ (3 \times 4)(3+4)(24mn - 8m - 8n + 4) \\
&+ (3 \times 5)(3+5)(12mn - 4m - 4n + 2) \\
&+ (4 \times 4)(4+4)(8mn - 4m) + (4 \times 5)(4+5)(8mn - 4m) \\
&= 5920mn - 1360m - 600n + 164
\end{aligned}$$

Table 7 and Figure 7 Provide both a Quantitative analysis and graphical depiction of $ReZG_1(MgAl_2O_4)$, $ReZG_2(MgAl_2O_4)$, $ReZG_3(MgAl_2O_4)$ respectively.

$[m, n]$	$ReZG_1(MgAl_2O_4)$	$ReZG_2(MgAl_2O_4)$	$ReZG_3(MgAl_2O_4)$
[1, 1]	38	78.87	4124
[2, 2]	132	351.35	19924
[3, 3]	282	818.67	47564
[4, 4]	488	1480.83	87044
[5, 5]	750	2337.83	138364
[6, 6]	1068	3389.67	201524
[7, 7]	1442	4636.35	276524
[8, 8]	1872	6077.87	363364
[9, 9]	2358	7714.23	462044
[10, 10]	2900	9545.43	572564

Table 7: Quantitative analysis $ReZG_1(MgAl_2O_4)$, $ReZG_2(MgAl_2O_4)$, $ReZG_3(MgAl_2O_4)$

The graph displays the redefined Zagreb indices $ReZG_1(MgAl_2O_4)$, $ReZG_2(MgAl_2O_4)$, and $ReZG_3(MgAl_2O_4)$ for the structure of magnesium aluminate $MgAl_2O_4$. The table shows the calculated results of these index for different set of $[m, n]$, thus both m and n fall between 1 to 10. It is sure that all three indices growing continuously and rapidly as

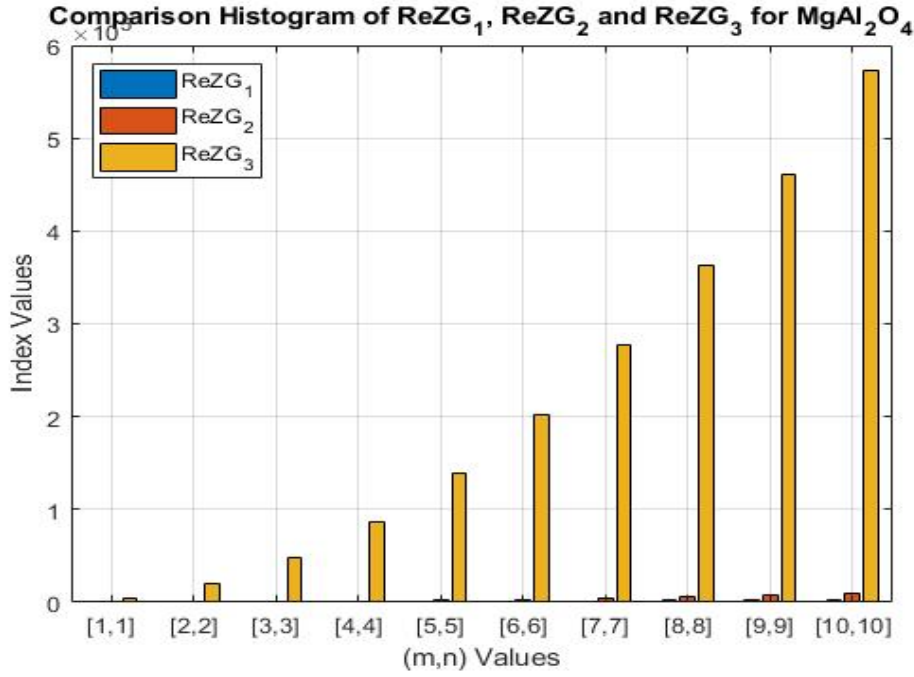


Figure 7: Graphical depiction $ReZG_1(MgAl_2O_4)$, $ReZG_2(MgAl_2O_4)$ and $ReZG_3(MgAl_2O_4)$

m and n grow up. The $ReZG_1$ values increase frequently from 38 at $[1, 1]$ to 2900 at $[10, 10]$, presenting a linear trend. On other hand, $ReZG_2$ growing more quickly, move from 78.87 to 9545.43, that show to a nonlinear connection. The $ReZG_3$ index display the most extreme grow up, rising from 4124 to 572564, presenting an exponential growth design. This general trend describe that the ReZG indices are fastly change by the values of $[m, n]$, with $ReZG_3$ being the very manner changes in the structure of $MgAl_2O_4$.

4 Investigation of heat of formation by Power interpolation

Curve fitting involves a statistical way to get a curve that best fits the connection specify by a set of data points. In particularly, one of the method is called power curve fitting. Power curve fitting can be an controlling tool in show the non-linear connection in scientific and mathematical data. Meaningful that what is the fitted variables or parameters (a, b, c) mean is necessary for explain the nature of the connection, evaluate system behavior, and making guess. It carry more information than would have been possible with simple linear models, as well as when modeling real life circumstance that naturally reveal power law behavior. In this work, we go in to power curve fitting as $mathfrak{P}_{cf}$. The enthalpy of formation (HOF) for magnesium aluminate ($MgAl_2O_4$) is estimated below using a power curve fitting model. [18, 19]. The enthalpy of formation, also specified heat of formation, is the thermodynamic characteristics of a given process that describe the change in enthalpy when one mole of the compound is create from its basic elements, which are generally in their standard states under standard conditions. These conditions usually mean a temperature of 298.15 K and a pressure of 1 atm [44]. Heat of formation calculated in the following way. All the value of HOF is provided in Table 8.

• Calculation of HOF

Standard enthalpy = -13.02 kJ/mol

Avogadro's No = 6.022×10^{23} mol⁻¹

$$\begin{aligned}
 HOF &= \frac{S.E}{AN} \\
 &= \frac{-13.02}{6.022 \times 10^{23}} \\
 HOF &= -2.162 \times 10^{-23}
 \end{aligned}$$

Table $[m, n]$	Unit $(m + n)^2$	Unit $\times HOF$	Result
[1, 1]	$(1 + 1)^2 = 4$	$4 \times -2.162 \times 10^{-23}$	-8.648×10^{-23}
[2, 2]	$(2 + 2)^2 = 16$	$16 \times -2.162 \times 10^{-23}$	-3.459×10^{-22}
[3, 3]	$(3 + 3)^2 = 36$	$36 \times -2.162 \times 10^{-23}$	-7.783×10^{-22}
[4, 4]	$(4 + 4)^2 = 64$	$64 \times -2.162 \times 10^{-23}$	-1.384×10^{-21}
[5, 5]	$(5 + 5)^2 = 100$	$100 \times -2.162 \times 10^{-23}$	-2.162×10^{-21}
[6, 6]	$(6 + 6)^2 = 144$	$144 \times -2.162 \times 10^{-23}$	-3.113×10^{-21}
[7, 7]	$(7 + 7)^2 = 196$	$196 \times -2.162 \times 10^{-23}$	-4.238×10^{-21}
[8, 8]	$(8 + 8)^2 = 256$	$256 \times -2.162 \times 10^{-23}$	-5.535×10^{-21}
[9, 9]	$(9 + 9)^2 = 324$	$324 \times -2.162 \times 10^{-23}$	-7.005×10^{-21}

Table 8: Heat of Formation (HOF) of ($MgAl_2O_4$)

In this study, a best-fit power function is used to describe the relationship between the indices and the corresponding heat of formation values. The indices are treated as the independent variable, denoted by x , while the heat of formation values are the dependent variable, denoted by y . The dataset is structured into two separate lists: one with the values of x and the other with the matching values of y . The power curve fitting method seeks to model this relationship with a function of the form

$$y = ax^b + c,$$

where a , b and c are variables or parameters to be determined. In particular, a denotes scaling factor, b is associated with nonlinear structural growth dynamics, and c stands for the baseline energetic value independent of the graph size. The fitting procedure is a numerical regression to determine the best guess of these parameters by the minimization of the sum of the squared differences between the actual observed values of y and what is predicted by the model. We start by considering a simple form of a power model and adjust its parameters to get the best fit to the data. This method results in a non-linear connection between the values of heat of formation and indices, hence giving a more approximate and illustrative relation.

$$y = ax + b.$$

The technique of linear regression curve fitting is a statistical approach that involves finding a relationship between an outcome variable and one or more predictor variables in the form of a straight line. Performance analysis of the suggested regression models will be conducted via statistical validation on the available sample set in the current research. Because the data sample set is very small in size, the suggested models will be tested and validated based on this single dataset. It uses a method of least squares to obtain the best-fit line. For estimate accuracy, a focusing check was performed, which was helped by statistical measures. Some of the most commonly used measures for assessing accuracy are (R^2), (SSE), and (RMSE). Graphical description on curve fitting are shown in Figure 8 - 21, and their individual measure could be introduced in Table 9 - 22.

In this work, the likelihood of trivial correlation due to an underlying shared dependence on graph size (or order) has been taken into account. To overcome this issue, we made sure that the topological indices chosen have both degree and normalized/co-index versions, and most are less sensitive to simple size scaling and more sensitive to finer structure variations in the $MgAl_2O_4$ network. Moreover, the correlation analysis was also supported with regression diagnostics where various models were tested and compared to ensure the predictive performance is not dependent only on the number of vertices or edges. Moreover, inter-descriptor correlation analysis was conducted to eliminate redundancy and prevent the effect of multicollinearity in the relationship with the size of the graph. The high correlation values obtained between structurally different configurations of similar order should also suggest that the predictive ability is due to the real relationship between the descriptors and the properties and not due to insignificant dependence on size. Therefore, the findings indicate that the topological descriptors used are effective in capturing structural characteristics that are important to the heat of formation, and not just the magnitude of the graph.

Our main aim in the current study is to determine an analytical relationship between the topological descriptors and the heat of formation of the network of $MgAl_2O_4$ by power curve fitting models. It focuses on understanding the innate structural sensitivity of degree-based topological indices and their potential to model thermodynamic behavior, instead of on predictive generalization using external validation schemes. The high pattern of correlation that is consistently present in the derived models depicts the high intrinsic correlation between the selected descriptors and the target property. As such, the nature of this work is oriented to theoretical modeling and structural interpretation, which gives a fundamental background to the studies in the future when long-term validation plans and predictive evaluations can be included.

• HOF using $R_1(MgAl_2O_4)$

Power model equation:

$$f(R_1) = (a \times x^b) + c$$

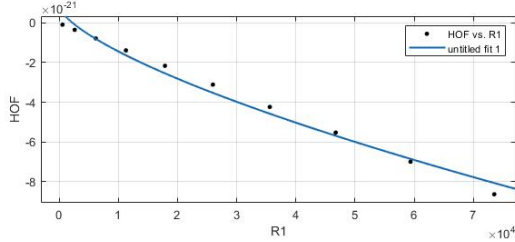
Linear model equation:

$$f(R_1) = ax + b$$

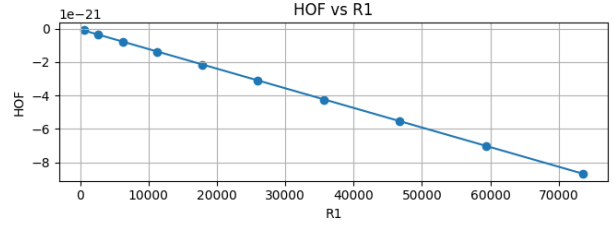
Table 9 based on the results of the model fitting, the coefficient a is about -3.934×10^{-24} , the exponent b is 0.6892, and the constant term c is 8.121×10^{-22} . These values show that the fitted curve shows a slowly increasing relationship, where the impact of x on $f(x)$ increases but not as quickly as x itself, because the exponent b is less than 1. The very small sizes of a and c suggest that the model predicts very small outputs across the entire range of x .

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$1.2826e-42$	0.9837	0.9790	$4.2805e-22$
Linear	$2.4768e-45$	0.9999	0.9988	$1.5737e-23$

Table 9: HOF and $R_1(MgAl_2O_4)$ by interpolation



(a) power2 model



(b) Linear model

Figure 8: $\mathfrak{P}_{cf}$ among HOF of $R_1(MgAl_2O_4)$

In Figure 8, the model fits the data very well, as shown by the high coefficient of determination $R^2 = 0.9837$ and the adjusted $R^2 = 0.979$, meaning about 98 percent of the changes in the data are explained by the model.

• HOF using $R_{-1}(MgAl_2O_4)$

Power model equation:

$$f(R_{-1}) = (a \times x^b) + c$$

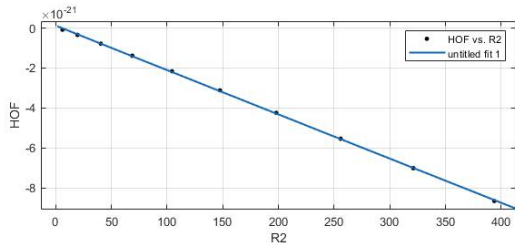
Linear model equation:

$$f(R_{-1}) = ax + b$$

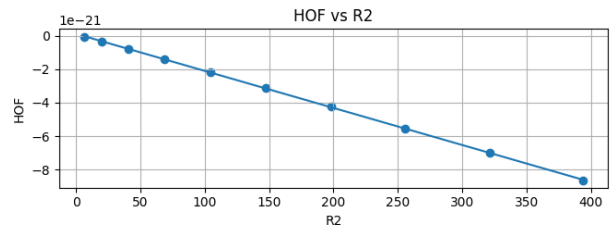
Table 10 based on the results from the curve fitting, the estimated parameters are $a = -2.266 \times 10^{-23}$, $b = 0.9961$, and $c = 1.222 \times 10^{-22}$. The exponent b is very close to 1, which suggests that the relationship between x and $f(x)$ is almost linear. The negative value of a along with the small positive constant c means that the function values stay extremely small throughout the data range.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$1.4330e-44$	0.9998	0.9998	$4.5256e-23$
Linear	$1.1513e-44$	0.9998	0.99987	$3.3931e-23$

Table 10: HOF and $R_{-1}(MgAl_2O_4)$ by interpolation .



(a) power2 model



(b) Linear model

Figure 9: $\mathfrak{P}_{cf}$ among HOF of $R_{-1}(MgAl_2O_4)$

In Figure 9 the model fits the data very well, as shown by the high coefficient of determination $R^2 = 0.9998$ and adjusted $R^2 = 0.9998$, meaning that over 99.9 percent of the variance in the data is explained by the model.

• HOF using $R_{\frac{1}{2}}(MgAl_2O_4)$

Power model equation:

$$f(R_{\frac{1}{2}}) = (a \times x^b) + c$$

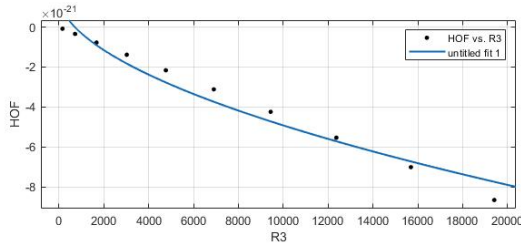
Linear model equation:

$$f(R_{\frac{1}{2}}) = ax + b$$

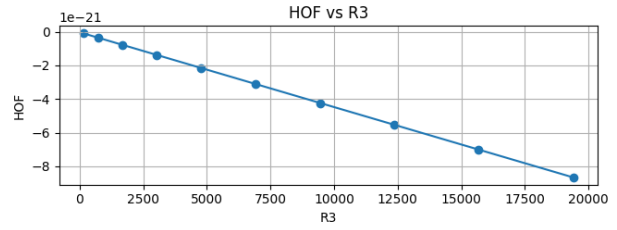
From the fitting results in Table 11, the coefficient a is -4.049×10^{-23} , the exponent b is 0.5499, and the constant term c is 1.492×10^{-21} . The value of $b < 1$ present the connection among x and $f(x)$ is sub-linear, define the function growing slowly as x increases. The small size of a and the relatively small constant c suggest that the function values stay very low across the dataset.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$3.1111 - 42$	0.9604	0.9491	$6.6667e - 22$
Linear	$8.6919e - 46$	0.9999	0.9998	$9.3230e - 24$

Table 11: HOF and $R_{\frac{1}{2}}(MgAl_2O_4)$ by interpolation .



(a) power2 model



(b) Linear model

Figure 10: $\mathfrak{P}_{cf}$ among HOF of $R_{\frac{1}{2}}(MgAl_2O_4)$

Figure 10 show visualization. The coefficient of determination $R^2 = 0.9604$ and adjusted $R^2 = 0.9491$ show that about 96% of the data variation is explained by the model, indicating a strong and dependable fit. Also, the low sum of squared errors ($SSE = 3.111 \times 10^{-42}$) and root mean square error ($RMSE = 6.667 \times 10^{-22}$) confirm that the actual and predicted values are very close.

• HOF using $R_{-\frac{1}{2}}(MgAl_2O_4)$

Power model equation:

$$f(R_{-\frac{1}{2}}) = (a \times x^b) + c$$

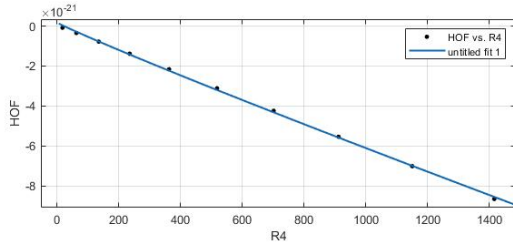
Linear model equation:

$$f(R_{-\frac{1}{2}}) = ax + b$$

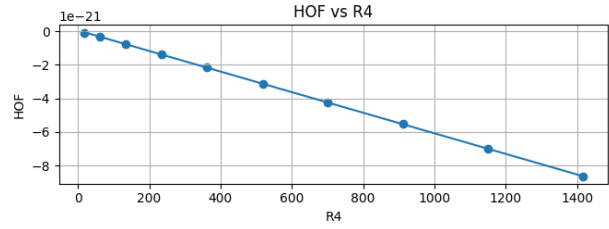
From the fitting results in Table 12, the parameter a is estimated to be -9.184×10^{-24} , the exponent b is 0.9448, and the constant term c is 1.707×10^{-22} . Since the exponent b is close to 1, the relationship between x and $f(x)$ is nearly linear. The very small magnitude of the coefficient a and constant term c indicates that the function values remain extremely small across the considered data range.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$5.2203e - 44$	0.9993	0.9991	$8.6358e - 23$
Linear	$1.8488e - 45$	0.9999	0.9997	$1.3597e - 23$

Table 12: HOF and $R_{-\frac{1}{2}}(MgAl_2O_4)$ by interpolation.



(a) power2 model



(b) Linear model

Figure 11: $\mathfrak{P}_{cf}$ among HOF of $R_{\frac{-1}{2}}(MgAl_2O_4)$

Figure 11 show graphical representation of HOF. The goodness-of-fit values further confirm the suitability of this model, with a high coefficient of determination $R^2 = 0.9993$ and adjusted $R^2 = 0.9991$, meaning that more than 99.9% of the variation in the observed data is explained by the model.

• **HOF using $ABC(MgAl_2O_4)$**

Power model equation:

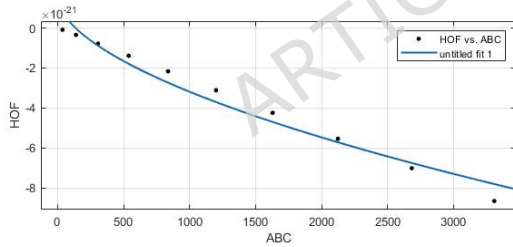
$$f(ABC) = (a \times x^b) + c$$

Linear model equation:

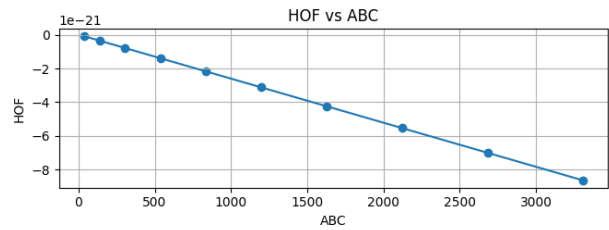
$$f(ABC) = ax + b$$

Table 13 Based on the fitting parameters, the coefficient a is -8.762×10^{-23} , the exponent b is 0.5752, and the constant term c is 1.472×10^{-21} . The value of b being less than 1 suggests a sub-linear growth pattern, meaning the function increases slowly as x increases. Both a and c have very small magnitudes, indicating that the predicted values of the function remain extremely small throughout the range of x .

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$2.7295e - 42$	0.9653	0.9554	$6.2445e - 22$
Linear	$3.8287e - 46$	0.9999	0.9995	$6.1876e - 24$

Table 13: HOF and $ABC(MgAl_2O_4)$ by interpolation.

(a) power2 model



(b) Linear model

Figure 12: $\mathfrak{P}_{cf}$ among HOF of $ABC(MgAl_2O_4)$

Figure 12 the goodness-of-fit measures show the model fits the data quite well, with a coefficient of determination $R^2 = 0.9653$ and an adjusted $R^2 = 0.9554$, which means about 96% of the variation in the observed data is explained by the model. Additionally, the small sum of squared errors ($SSE = 2.73 \times 10^{-42}$) and root mean square error ($RMSE = 6.244 \times 10^{-22}$) show that the difference between the experimental and fitted values is minimal. Therefore, the General Power model offers a reliable and acceptable description of the dataset.

• **HOF using $GA(MgAl_2O_4)$**

Power model equation:

$$f(GA) = (a \times x^b) + c$$

Linear model equation:

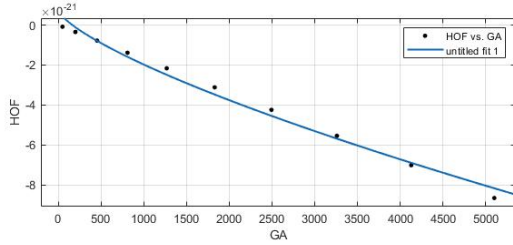
$$f(GA) = ax + b$$

From the curve fitting results in Table 14, the coefficient a is -1.14×10^{-23} , the exponent b is 0.7791, and the constant term c is 5.587×10^{-22} . Since the exponent b is less than 1, this indicates a sub-linear relationship between x and

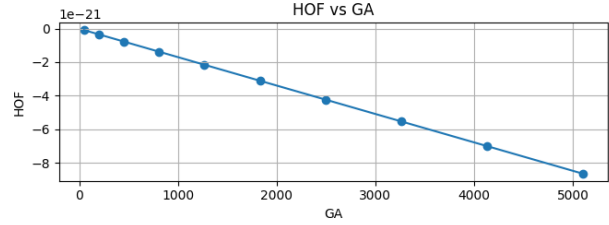
$f(x)$, meaning that the function increases gradually as x increases. The very small magnitudes of a and c suggest that the predicted output values remain very small throughout the dataset.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$9.5952e - 43$	0.9878	0.9843	$3.7023e - 22$
Linear	$1.1057e - 46$	0.9999	0.9998	$3.3253e - 24$

Table 14: HOF and $GA(MgAl_2O_4)$ by interpolation.



(a) power2 model



(b) Linear model

Figure 13: $\mathfrak{P}_c f$ among HOF of $GA(MgAl_2O_4)$

In Figure 13 the model exhibits a strong goodness of fit, as reflected by the coefficient of determination $R^2 = 0.992$ and adjusted $R^2 = 0.9898$, which show that approximately 99% of the data variation is explained by the model. Furthermore, the low sum of squared errors ($SSE = 6.263 \times 10^{-43}$) and the small root mean square error ($RMSE = 2.991 \times 10^{-22}$) confirm that the differences between the observed and fitted values are minimal. Therefore, the General Power model provides an accurate and reliable fit to the experimental data.

• HOF using $M_1(MgAl_2O_4)$

Power model equation:

$$f(M_1) = (a \times x^b) + c$$

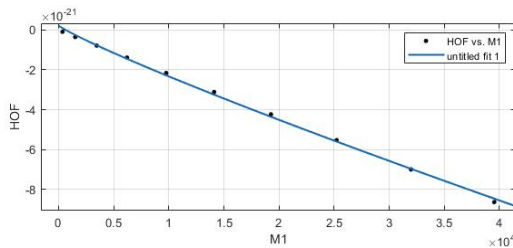
Linear model equation:

$$f(M_2) = ax + b$$

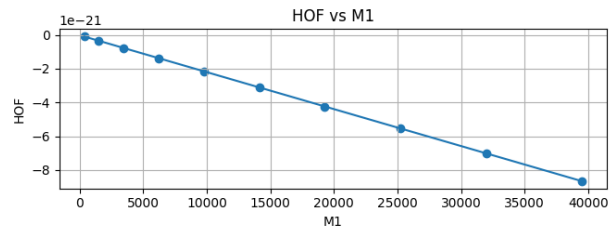
From the model's fitting results in Table 15, the coefficient a is -6.985×10^{-25} , the exponent b is 0.8909, and the constant term c is 2.282×10^{-22} . Because the exponent b is less than 1, the model shows a sub-linear relationship between the variable x and the function $f(x)$, meaning that as x increases, the function grows but at a slower and slower rate. The very small values of a and c suggest that the function's output stays nearly unchanged across the range of input values.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$1.2085e - 43$	0.9983	0.9979	$1.3620e - 22$
Linear	$4.6241e - 46$	0.9999	0.9993	$6.8001e - 24$

Table 15: HOF and $M_1(MgAl_2O_4)$ by interpolation.



(a) power2 model



(b) Linear model

Figure 14: $\mathfrak{P}_c f$ among HOF of $M_1(MgAl_2O_4)$

The model fits the data very well show in Figure 14, with a high coefficient of determination $R^2 = 0.9983$ and an adjusted $R^2 = 0.9979$, which means that more than 99.8Furthermore, the low sum of squared errors ($SSE =$

1.299×10^{-43}) and the small root mean square error ($\text{RMSE} = 1.362 \times 10^{-22}$) show that the differences between the actual and predicted values are very tiny, confirming that the model's predictions closely match the observed data.

• **HOF using $M_2(\text{MgAl}_2\text{O}_4)$**

Power model equation:

$$f(M_2) = (a \times x^b) + c$$

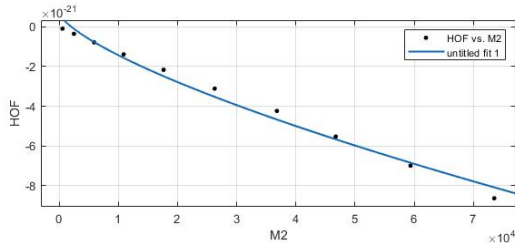
Linear model equation:

$$f(M_2) = ax + b$$

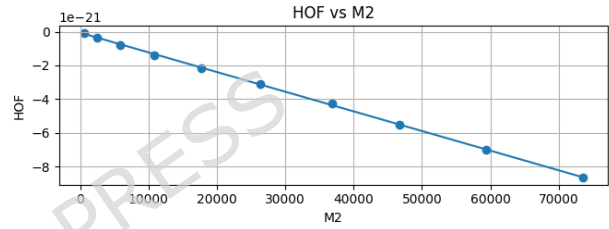
Based on the fitting results in Table 16, the coefficient a was found to be -2.99×10^{-24} , the exponent b is 0.7127, and the constant term c is 6.95×10^{-22} . Because the exponent b is less than 1, this suggests a sub-linear growth pattern, meaning that the function increases at a decreasing rate as x increases. The very small values of a and c indicate that the predicted function values stay close to zero across the entire range of the data.

Fit - type	SSE	r^2	$\text{adj}(r^2)$	RMSE
power2	$1.6224e - 42$	0.9852	0.9810	$4.0751e - 22$
Linear	$2.1413e - 44$	0.9997	0.9996	$4.6274e - 23$

Table 16: HOF and $M_2(\text{MgAl}_2\text{O}_4)$ by interpolation.



(a) power2 model



(b) Linear model

Figure 15: $\mathfrak{P}_c f$ among HOF of $M_2(\text{MgAl}_2\text{O}_4)$

The model fits the data very well show in Figure 15, as evidenced by the high coefficient of determination, $R^2 = 0.9852$, and the adjusted $R^2 = 0.981$, which means that around 98% is accounted for by the model. Additionally, the low sum of squared errors ($\text{SSE} = 1.162 \times 10^{-42}$) and the small root mean square error ($\text{RMSE} = 4.075 \times 10^{-22}$) show that the difference between the actual and predicted values is minimal. Consequently, the General Power model offers a precise and dependable description of the dataset.

• **HOF using $HM(MgAl_2O_4)$**

Power model equation:

$$f(HM) = (a \times x^b) + c$$

Linear model equation:

$$f(HM) = ax + b$$

From the curve fitting results in Table 17, the coefficient a is -9.26×10^{-24} , the exponent b is 0.547, and the constant term c is 1.506×10^{-21} . Since the exponent $b < 1$, the model indicates a sub-linear relationship, meaning that the function increases slowly as x increases. The very small magnitudes of a and c suggest that the predicted function values remain extremely small over the input range.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$3.1188e - 42$	0.9603	0.9490	$6.6749e - 22$
Linear	$1.4315e - 45$	0.9999	0.9998	$1.1964e - 23$

Table 17: HOF and $HM(MgAl_2O_4)$ by interpolation.

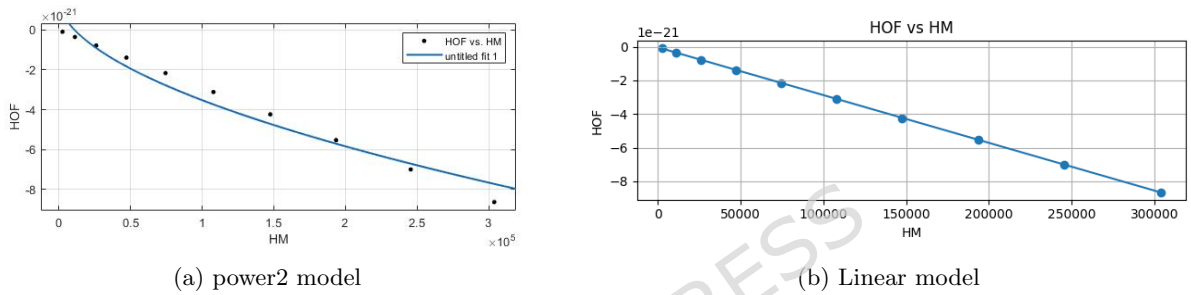


Figure 16: $\mathfrak{P}_cf$ among HOF of $HM(MgAl_2O_4)$

The goodness of fit is reflected by the coefficient of determination $R^2 = 0.9603$ and the adjusted $R^2 = 0.949$, showing that approximately 96% of the variation in the data is explained by the model shown in Figure 16. Additionally, the low sum of squared errors ($SSE = 3.119 \times 10^{-42}$) and the root mean square error ($RMSE = 6.675 \times 10^{-22}$) indicate small residual differences between the observed and predicted values. Therefore, the General Power model provides a reasonably accurate and reliable representation of the dataset.

• **HOF using $PM_1(MgAl_2O_4)$**

Power model equation:

$$f(PM_1) = (a \times x^b) + c$$

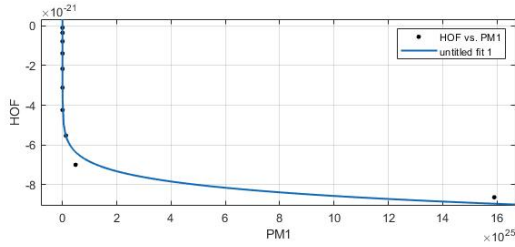
Linear model equation:

$$f(PM_1) = ax + b$$

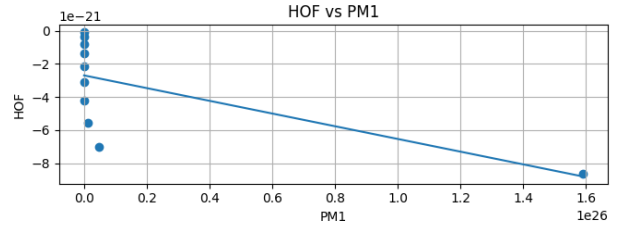
From the fitting results in Table 18, the coefficient a is -6.699×10^{-23} , the exponent b is 0.08347, and the constant term c is 1.333×10^{-21} . The very small value of the exponent b , which is close to zero, indicates that the function changes very slowly with respect to x , suggesting an almost constant behavior across the dataset. The small magnitude of a and the relatively small value of c further indicate that the predicted function values remain extremely small throughout the domain.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	2.1146	0.9731	0.9654	$5.4962e - 22$
Linear	$4.5282e - 41$	0.4226	0.3505	$2.1303e - 21$

Table 18: HOF and $PM_1(MgAl_2O_4)$ by interpolation .



(a) power2 model



(b) Linear model

Figure 17: $\mathfrak{P}_c f$ among HOF of $PM_1(MgAl_2O_4)$

The model demonstrates a strong goodness of fit, with a coefficient of determination $R^2 = 0.9731$ and adjusted $R^2 = 0.9654$, showing that approximately 97% of the variation in the observed data is explained by the model presented visually in Figure 17. Additionally, the low sum of squared errors ($SSE = 2.115 \times 10^{-42}$) and root mean square error ($RMSE = 5.496 \times 10^{-22}$) confirm that the residual differences between the observed and predicted values are minimal. Therefore, the General Power model provides a reliable and accurate representation of the dataset.

• **HOF using $PM_2(MgAl_2O_4)$**

Power model equation:

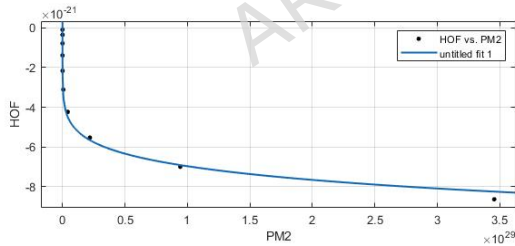
$$f(PM_2) = (a \times x^b) + c$$

Linear model equation:

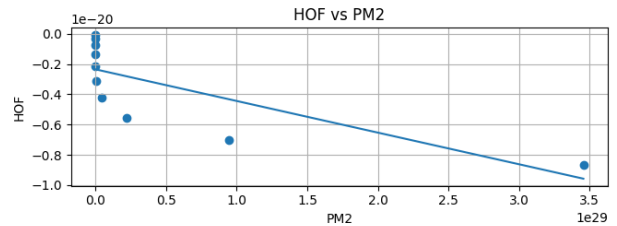
$$f(PM_2) = ax + b$$

Table 19 based on the estimated parameters, the coefficient a is -1.444×10^{-24} , the exponent b is 0.128, and the constant term c is 4.712×10^{-22} . Given that the exponent b is near zero, the model suggests that the function changes very gradually with respect to x , indicating an almost constant trend across the data range. The extremely small values of both a and c mean that the predicted function values are also very small.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$6.1071e-43$	0.9922	0.9900	$2.9537e-22$
Linear	$3.1884e-41$	0.5943	0.5436	$1.7856e-21$

Table 19: HOF and $PM_2(MgAl_2O_4)$ by interpolation .

(a) power2 model



(b) Linear model

Figure 18: $\mathfrak{P}_c f$ among HOF of $PM_2(MgAl_2O_4)$

The model exhibits a high level of fit, as shown by $R^2 = 0.9922$ and adjusted $R^2 = 0.99$, which means that about 99% of the variation in the observed data is accounted for by the model in Figure 18. Furthermore, the low sum of squared errors ($SSE = 6.107 \times 10^{-43}$) and the root mean square error ($RMSE = 2.954 \times 10^{-22}$) confirm that the differences between the actual and predicted values are very small. Overall, the General Power model offers a precise and dependable description of the dataset.

• **HOF using $ReZG_1(MgAl_2O_4)$**

Power model equation:

$$f(ReZG_1) = (a \times x^b) + c$$

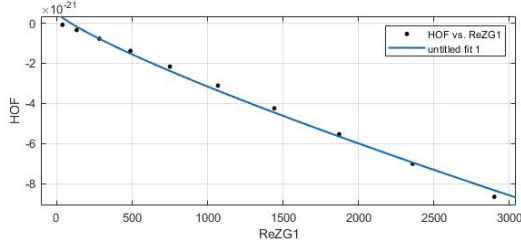
Linear model equation:

$$f(ReZG_2) = ax + b$$

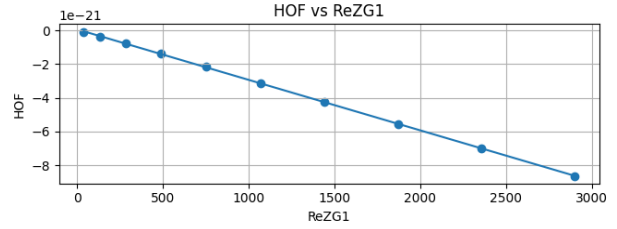
From the fitting results in Table 20, the estimated parameters are $a = -1.236 \times 10^{-23}$, $b = 0.8244$, and $c = 5.175 \times 10^{-22}$. Since the exponent b is less than 1, this indicates a sub-linear relationship, meaning that the function increases slowly as x increases. The very small magnitudes of the parameters a and c imply that the function values remain extremely small throughout the domain.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$4.5252e - 43$	0.9942	0.9926	$2.5426e - 22$
Linear	$3.7029e - 45$	0.9995	0.9994	$1.9242e - 23$

Table 20: HOF and $ReZG_1(MgAl_2O_4)$ by interpolation.



(a) power2 model



(b) Linear model

Figure 19: $\mathfrak{P}_cf$ among HOF of $ReZG_1(MgAl_2O_4)$

The model exhibits a strong goodness of fit, with a coefficient of determination $R^2 = 0.9942$ and adjusted $R^2 = 0.9926$, showing that more than 99% of the variation in the observed data is explained by the model shown in Figure 19. Additionally, the small sum of squared errors ($SSE = 4.525 \times 10^{-43}$) and the low root mean square error ($RMSE = 2.543 \times 10^{-22}$) indicate that the discrepancies between the observed and fitted values are minimal. Therefore, the General Power model provides a highly accurate and reliable representation of the dataset.

• HOF using $ReZG_2(MgAl_2O_4)$

Power model equation:

$$f(ReZG_2) = (a \times x^b) + c$$

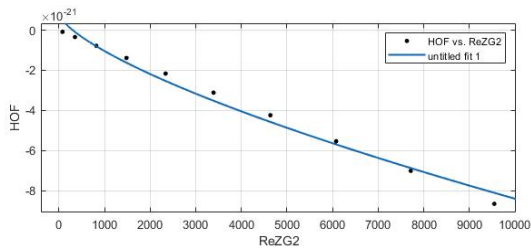
Linear model equation:

$$f(ReZG_2) = ax + b$$

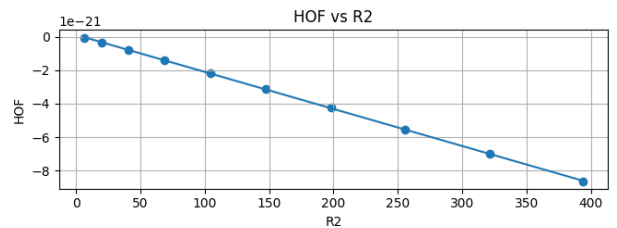
Table 21 Based on the results of the analysis, the estimated values for the parameters are $a = -1.457 \times 10^{-23}$, $b = 0.6999$, and $c = 7.933 \times 10^{-22}$. Because the exponent b is less than 1, the model shows that the function grows in a sub-linear way, meaning it increases slowly as x increases. The very small values of the coefficients a and c suggest that the function values remain nearly unchanged and very small across the range of the data.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$1.19863 - 42$	0.9848	0.9804	$4.1381e - 22$
Linear	$1.3348e - 45$	0.9999	0.9998	$1.15753e - 23$

Table 21: HOF and $ReZG_2(MgAl_2O_4)$ by interpolation .



(a) power2 model



(b) Linear model

Figure 20: $\mathfrak{P}_cf$ among HOF of $ReZG_2(MgAl_2O_4)$

The model fits the data very well, as shown in Figure 20 by the high coefficient of determination $R^2 = 0.9848$ and the adjusted $R^2 = 0.9804$, which means the model explains about 98% of the variation in the observed data. Additionally,

the low sum of squared errors ($SSE = 1.199 \times 10^{-42}$) and the root mean square error ($RMSE = 4.138 \times 10^{-22}$) confirm that the difference between the actual data points and the model's predictions is very small. Therefore, the General Power model is both accurate and dependable for representing the dataset.

• **HOF using $ReZG_3(MgAl_2O_4)$**

Power model equation:

$$f(ReZG_3) = (a \times x^b) + c$$

Linear model equation:

$$f(ReZG_3) = ax + b$$

According to the fitting results in Table 22, the coefficient a is -6.456×10^{-25} , the exponent b is 0.7184, and the constant term c is 6.885×10^{-22} . Since the exponent b is less than 1, the relationship between x and $f(x)$ is sub-linear, meaning that the function increases slowly as x increases. The very small magnitudes of a and c indicate that the predicted function values remain extremely small throughout the range of the data.

Fit - type	SSE	r^2	$adj(r^2)$	RMSE
power2	$1.0084e - 42$	0.9872	0.9835	$3.7955e - 22$
Linear	$3.6183e - 45$	0.9999	0.9994	$1.9022e - 23$

Table 22: HOF and $ReZG_3(MgAl_2O_4)$ by interpolation.

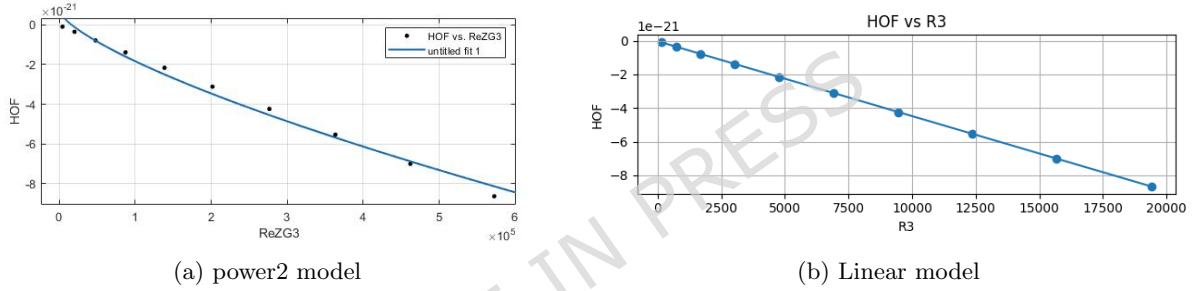


Figure 21: $\mathfrak{P}_cf$ among HOF of $ReZG_3(MgAl_2O_4)$

The goodness-of-fit measures show that the model fits the data very well, with a coefficient of determination $R^2 = 0.9872$ and an adjusted $R^2 = 0.9835$, implying that approximately 98% of the variation in the observed data is explained by the model in Figure 21. Furthermore, the low sum of squared errors ($SSE = 1.008 \times 10^{-42}$) and the small root mean square error ($RMSE = 3.795 \times 10^{-22}$) confirm that the residuals between the observed and predicted values are minimal. Therefore, the General Power model provides a reliable and accurate representation of the dataset.

5 Comparison of Model Performance

Index	GA	ABC	M1	R3	ReZG2	HM	R4	R1	ReZG3	ReZG1	R2	M2	PM2	PM1
Linear	0.999999	0.999995	0.999994	0.999989	0.999983	0.999982	0.999976	0.999968	0.999954	0.999953	0.999854	0.999728	0.59439	0.422677
Power	0.9878	0.9653	0.9983	0.9604	0.9848	0.9603	0.9993	0.9837	0.9835	0.9942	0.9998	0.9852	0.9922	0.9731

Table 23: Comparison of Linear and Power model R^2 values

Figure 22 and Table 23 shows a comparison between the two models: Linear Regression and Power Regression. The chart depicts the coefficient of determination (R^2) values for fourteen separate indices. Until indices GA to M2, the Linear model displays a perfectly accurate prediction with an unvarying R^2 of 1.0, barely marginally beating the other one that falls between 0.96 and 1.0. A drastic change occurs starting from index PM2 onwards, where the Linear model performs poorly with an approximate value of 0.59, while at PM1, its score drops drastically to 0.42. Conversely, the Power model shows a greater degree of reliability in these latter parts with an approximate R^2 of 0.98.

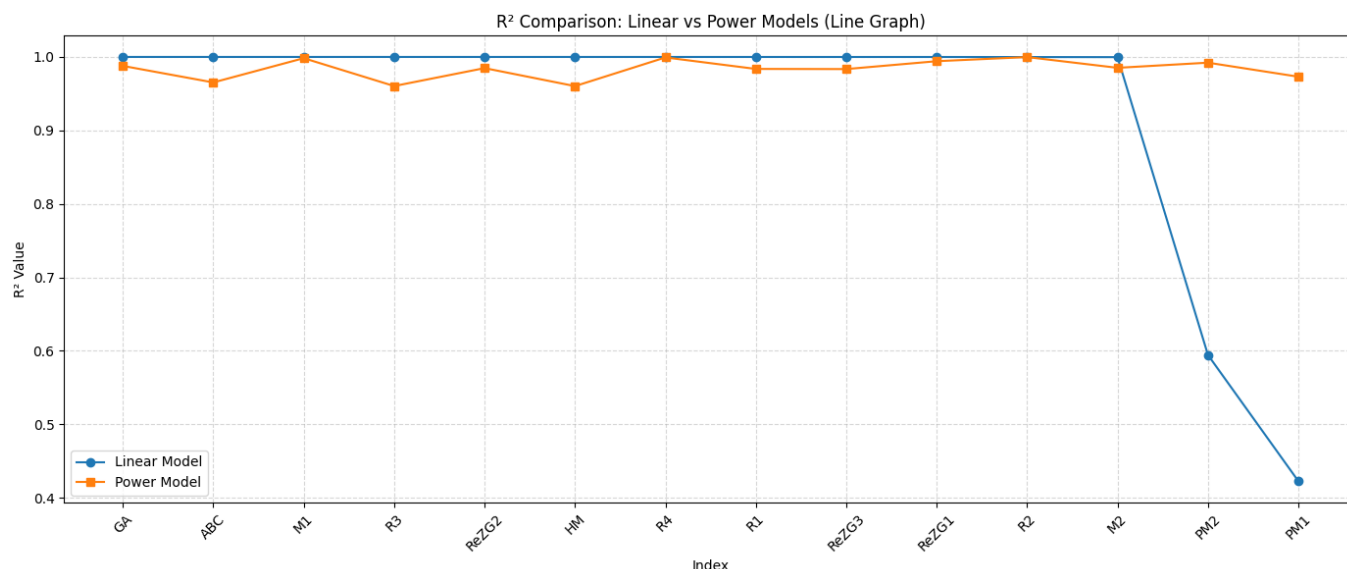


Figure 22: Graphical visualization of Comparison

6 Conclusion

In this paper, an interpolation model was used to closely examine how topological indices relate to the heat of formation in a network of Magnesium aluminate ($MgAl_2O_4$). First, the topological indices of ($MgAl_2O_4$) were calculated using edge partitioning based on vertex degrees. Then, the heat of formation for Magnesium aluminate was calculated by numerical computations carried out using MATLAB; similarly, the graphs were also draw in the same software.

A power curve fitting model appropriate the statistics using MATLAB and present the best connection than when easy polynomial models were used. The examination followed the tendency of difference of topological indices with respect to the *HOF* in the ($MgAl_2O_4$) network. Visualization showed the trends of variation, together with particular index values where variation in heat of formation were notable. The heat of formation was found to be nearly linked to various topological indices in the network of ($MgAl_2O_4$). This indicate that topological indices can work as valid tools for producing guess about thermodynamic properties and offer useful observation into their use in studies involving molecular networks and similar systems.

These discovery point to a number of potentially useful path for further research. One such path associate the addition of the present methodology to other types of nanostructures, such as transition metal carbides, nitrides, or boron-based nanostructures, in order to research if similar connection take place in different chemical systems. Such relative studies will also support in clarifying the prescient capacity of topological indices outside of ($MgAl_2O_4$) system. One more path is the union of amount of chemical simulations with topological indices, which can refer more specific models, together with atomic orbital information.

More preciously, this research, the interpolation method of modeling has been employed to explore the connection between topological indices and the heat of formation (HOF) of the Magnesium aluminate ($MgAl_2O_4$). Firstly, degree-based topological indices have been determined by partitioning the graph edges. The HOF values have then been calculated numerically using MATLAB. The correlation between topological indices and heat of formation (HOF) of ($MgAl_2O_4$) were studied using the linear and power functions. It can be observed that the performance of the linear function for the majority of the indices is better than the power function with R^2 values being higher, and the power function outperformed in a few instances of indices. These results suggest that combining linear and nonlinear models offers a more comprehensive understanding and can be extended to other structures for future research.

Data Availability

The datasets used and/or analysed during the current study available from the corresponding author on reasonable request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Funding statement

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Authors Contributions

Sadia Nazir was involved in the Computation, and analysis of the paper and also assent to the final adumbrate of the paper. Muhammad Kamran Siddiqui contributed to Elevating the graphs of maple and Matlab calculations, supervised the project, Envisioned it, Organized the methodology, coordinated it, found resources, and wrote the starting adumbrate of the paper. For investigating, analyzing data Creation, and designing experiments Hasnain Hayat worked. Brima Gegbe works on software development, validation, funding acquisition, and formal analysis of studies. Every author reviews and approves the final report of the work.

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