Research Article

On Analysis of Topological Properties for Terbium IV Oxide via Enthalpy and Entropy Measurements

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A relation between topological indices and thermodynamics properties of terbium IV oxide has been established by using a rational method as it was found the most efficient method based on mean squared error (MSE). Terbium IV oxide has huge application as an insulator in modern technologies such as microelectronics, gas detectors, and luminiferous owing to mechanical and thermal stability, high dielectric constant, radiation resistance, and variable electrical conductivity. The chemical graph and topological indices have attracted the research community due to their potential application in discrete mathematics, biology, and chemistry. Our commitment is to investigate topological indices and thermodynamic properties of terbium IV oxide that depend on an innovative data utilitarian. Moreover, a relationship between topological indices and curve fitting has been established as an application point of view. All curve fittings have been found using MATLAB software.

1. Introduction

Terbium, a rare earth metal, is a member of the 4f series of the periodic table called lanthanides and has electronic configuration $[\text{Xe}] 4f^9 6s^2$. It is found between the $(n-1)d$ and ns block elements and has properties identical to d-block elements. Due to unfilled f orbital, electrons are added to the $(n-2)$ level's 'f' suborbitals. It is silvery white soft metal with a silvery appearance whose melting point ranges from 1000 to 1200 degrees Celsius and is an excellent heat and electricity conductor. Except for promethium, lanthanides are nonradioactive in nature [1, 2]. The synthesis of terbium IV oxide conventionally uses the precipitation approach, but newly designed self-propagation high-temperature synthesis (SHS) provides the high yield of weakly agglomerated nanosized powder of terbium IV oxide. The flow sheet of this process is given in Figures 1 and 2 [3].

Terbium IV oxide films have huge application as an insulator in microelectronics, gas detectors, and

luminophores due to unique properties such as radiation resistance and very small leakage current density besides variable electrical conductivity in different gaseous fluids [4, 5]. It is found that various oxidation states cause changes in the stoichiometry of terbium IV oxide that predetermines variations in its optical properties, thus making it useful for the aforementioned applications as well as in Fresnel lenses, pigments, antireflection layers, and photoelastic films [6, 7]. Terbium compounds are brightly fluorescent, and most terbium supplies are used to produce green phosphorous worldwide that allow trichromatic lighting [8]. It is also often used as a dopant for fuel-cell materials and crystalline solid-state devices. The large surface basicity, rapid oxygen ion mobility, and interesting catalytic characteristics of earth oxides are well known. These are the qualities which make them a good chemical sensor [9].

The bulk structure of TbO_2 is crystallized as a Tb_4O_8 . In a crystal of terbium oxide, oxygen atoms are located in the cubic closed packed terbium atoms (Figure 1) [10].

FIGURE 1: Schematic illustration of terbium IV oxide synthesis of by SHS.

FIGURE 2: Unit cell structure of terbium oxide [4].

Metal oxide redox reactions are currently regarded being one of the most favorable long-term methods for producing renewable H_2 for immediate use in fuel cells. Terbium IV oxide is a promising candidate for thermochemical production of hydrogen through solar thermochemical water splitting (Tb-WS) cycle. The first step of the cycle includes the thermal reduction of TbO_2 into Tb and O_2 , while the second step involves oxidation of Tb through a water splitting reaction to produce H_2 . The unit cell structure of terbium oxide is depicted in Figure 2.

Step 1. Step 1:

Equation (1) is the endothermic reduction.

Step 2.

Equation (2) is the endothermic reduction.

2. Degree-Based Topological Indices

Let $G = (V, E)$ be a graph where V is the vertex set and E is the edge set of G . The degree $\tilde{I}(a)$ of a vertex a is the number of edges of G incident with a .

In 2013, Shirdel et al. [11] introduced the “Hyper-Zagreb index”:

$$HM = HM(G) = \sum_{ab \in E(G)} [\tilde{I}(a) + \tilde{I}(b)]^2. \quad (3)$$

In 2012, Ghorbani and Azimi [12] defined multiple Zagreb indices as

$$\begin{aligned} PM_1(G) &= \prod_{ab \in E(G)} [\tilde{I}(a) + \tilde{I}(b)], \\ PM_2(G) &= \prod_{ab \in E(G)} [\tilde{I}(a) + \tilde{I}(b)]. \end{aligned} \quad (4)$$

For more details about these indices, see [13, 14].

In 1972, Furtula and Gutman [15, 16] presented the forgotten topological index which was characterized as

$$F(G) = \sum_{ab \in E(G)} (\tilde{I}(a)^2 + \tilde{I}(b)^2). \quad (5)$$

Furtula et al. [17] introduced the “augmented Zagreb index”:

$$AZI(G) = \sum_{ab \in E(G)} \left(\frac{\tilde{I}(a) \times \tilde{I}(b)}{\tilde{I}(a) + \tilde{I}(b) - 2} \right)^3. \quad (6)$$

The Balaban index [18, 19] is a topological index based on order n and size m of graph G :

$$J(G) = \frac{m}{m - n + 2} \sum_{ab \in E(G)} \frac{1}{\sqrt{\tilde{I}(a) \times \tilde{I}(b)}}, \quad (7)$$

where $\tilde{I}(a), \tilde{I}(b)$ are the degrees of the vertices $a, b \in V(G)$.

For more details about these indices, see [20–22].

The redefined version of the Zagreb indices was defined by Ranjini et al. [23].

$$\begin{aligned} ReZG_1(G) &= \sum_{ab \in E(G)} \frac{\tilde{I}(a) + \tilde{I}(b)}{\tilde{I}(a) \times \tilde{I}(b)}, \\ ReZG_2(G) &= \sum_{ab \in E(G)} \frac{\tilde{I}(a) \times \tilde{I}(b)}{\tilde{I}(a) + \tilde{I}(b)}, \end{aligned} \quad (8)$$

$$ReZG_3(G) = \sum_{ab \in E(G)} \tilde{I}(a) \times \tilde{I}(b) (\tilde{I}(a) + \tilde{I}(b)).$$

For more details about these indices, see [24–31].

3. Results for Terbium Oxide (TbO_2)

The number of vertices and edges of the structure of terbium oxide denoted by (TbO_2) are 22 mn and 32 mn, respectively. There are three type of vertices in TbO_2 , namely, the vertices of degree 1, 2, and 4, respectively. The vertex partition of the

vertex set TbO_2 is presented in Table 1. Also, the edge partition of TbO_2 based on degrees of end vertices of each edge is depicted in Table 2.

(i) The Hyper-Zagreb index:

$$\begin{aligned}
 HM(G) &= \sum_{ab \in E(G)} (\tilde{I}(a) + \tilde{I}(b))^2, \\
 &= \sum_{ab \in E_1(G)} (\tilde{I}(a) + \tilde{I}(b))^2 + \sum_{ab \in E_2(G)} (\tilde{I}(a) + \tilde{I}(b))^2 + \sum_{ab \in E_3(G)} (\tilde{I}(a) + \tilde{I}(b))^2, \\
 &= HM(G) = (12mn - 2n - 2m)(1 + 4)^2 + (4mn - 2m - 2n)(2 + 4)^2 \\
 &\quad + (16mn + 4m + 4n)(4 + 4)^2, \\
 &= HM(G) = 4540mn + 902m + 902n.
 \end{aligned} \tag{9}$$

(ii) The first and second multiplicative Zagreb index:

The first multiplicative Zagreb index is computed as

$$\begin{aligned}
 PM_1(G) &= (1 + 4)^{(12mn - 2n - 2m)} \cdot (2 + 4)^{(4mn - 2m - 2n)} \cdot (4 + 4)^{(16mn + 4m + 4n)}, \\
 PM_1(G) &= 5^{(12mn - 2n - 2m)} \cdot 6^{(4mn - 2m - 2n)} \cdot 8^{(16mn + 4m + 4n)}, \\
 PM_1(G) &= \prod_{ab \in E(G)} (\tilde{I}(a) + \tilde{I}(b)) = \prod_{ab \in E_1(G)} (\tilde{I}(a) + \tilde{I}(b)) + \prod_{ab \in E_2(G)} (\tilde{I}(a) + \tilde{I}(b)) + \prod_{ab \in E_3(G)} (\tilde{I}(a) + \tilde{I}(b)).
 \end{aligned} \tag{10}$$

The second multiplicative Zagreb index is computed as

$$\begin{aligned}
 PM_2(G) &= \prod_{ab \in E(G)} ((\tilde{I}(a) + \tilde{I}(b))) = \prod_{ab \in E_1(G)} (\tilde{I}(a) + \tilde{I}(b)) + \prod_{ab \in E_2(G)} (\tilde{I}(a) + \tilde{I}(b)) + \prod_{ab \in E_3(G)} (\tilde{I}(a) + \tilde{I}(b)), \\
 PM_2(G) &= (1 + 4)^{(12mn - 2n - 2m)} \cdot (2 + 4)^{(4mn - 2m - 2n)} \cdot (4 + 4)^{(16mn + 4m + 4n)}, \\
 PM_2(G) &= 4^{(12mn - 2n - 2m)} \cdot 8^{(4mn - 2m - 2n)} \cdot 16^{(16mn + 4m + 4n)}.
 \end{aligned} \tag{11}$$

(iii) The first and second multiplicative Zagreb index:

The numerical representation of the above computed results is presented in Table 3.

(iv) The forgotten index:

The forgotten index is computed as

$$\begin{aligned}
 F(G) &= \sum_{ab \in E(G)} (\tilde{I}(a)^2 + \tilde{I}(b)^2), \\
 &= F(G) = \sum_{ab \in E_1} [\tilde{I}(a)^2 + \tilde{I}(b)^2] + \sum_{ab \in E_2} [\tilde{I}(a)^2 + \tilde{I}(b)^2] + \sum_{ab \in E_3} [\tilde{I}(a)^2 + \tilde{I}(b)^2], \\
 &= (12mn - 2n - 2m)((1)^2 + (4)^2) + (4mn - 2m - 2n)((2)^2 + (4)^2) + (16mn + 4m + 4n)((4)^2 + (4)^2), \\
 &= (12mn - 2n - 2m)(17) + (4mn - 2m - 2n)(20) + (16mn + 4m + 4n)(32) \\
 &\quad \cdot 796mn + 54m + 54n.
 \end{aligned} \tag{12}$$

TABLE 1: Vertex partition of TbO_2 based on the degree of vertex.

$\tilde{I}(a)$	Frequency	Set of vertices
1	$4mn + 4$	V_1
2	$2n + 2m - 4$	V_2
4	$18mn - 2m - 2n$	V_3

TABLE 2: Edge partition of TbO_2 .

$(\tilde{I}(a), \tilde{I}(b))$	Frequency	Set of edges
(1, 4)	$12mn - 2n - 2m$	E_1
(2, 4)	$4mn - 2m - 2n$	E_2
(4, 4)	$16mn + 4m + 4n$	E_3

TABLE 3: Comparison of indices $\text{HM}(G)$, PM_2 , $\text{PM}_2(G)$.

$[m, n]$	$\text{HM}(G)$	$\text{PM}_1(G)$	$\text{PM}_2(G)$
[1, 1]	6344	1.844×10^{27}	$5.192296859 \times 10^{33}$
[2, 2]	21768	2.699×10^{106}	$4.332296397 \times 10^{127}$
[3, 3]	46272	3.132×10^{237}	$5.808659799 \times 10^{281}$
[4, 4]	79856	2.883×10^{420}	$1.251505764 \times 10^{496}$
[5, 5]	122520	2.105×10^{655}	$4.333002103 \times 10^{770}$
[6, 6]	174264	1.219×10^{942}	$2.410705053 \times 10^{1105}$
[7, 7]	235088	5.600×10^{1280}	$2.155253650 \times 10^{1500}$

The Augmented Zagreb index is computed as follows:

(v) The Augmented Zagreb index:

$$\begin{aligned}
 \text{AZI}(G) &= \sum_{ab \in E(G)} \left(\frac{\tilde{I}(a) \times \tilde{I}(b)}{\tilde{I}(a) + \tilde{I}(b) - 2} \right)^3, \\
 \text{AZI}(G) &= \sum_{ab \in E_1} \left(\frac{\tilde{I}(a) \times \tilde{I}(b)}{\tilde{I}(a) + \tilde{I}(b) - 2} \right)^3 + \sum_{ab \in E_2} \left(\frac{\tilde{I}(a) \times \tilde{I}(b)}{\tilde{I}(a) + \tilde{I}(b) - 2} \right)^3 + \sum_{ab \in E_3} \left(\frac{\tilde{I}(a) \times \tilde{I}(b)}{\tilde{I}(a) + \tilde{I}(b) - 2} \right)^3, \\
 &= \sum_{ab \in E_1} \left(\frac{1 \times 4}{1 + 4 - 2} \right)^3 + \sum_{ab \in E_2} \left(\frac{2 \times 4}{2 + 4 - 2} \right)^3 + \sum_{ab \in E_3} \left(\frac{4 \times 4}{4 + 4 - 2} \right)^3, \\
 &= \frac{64}{27} (12mn - 2n - 2m) + 8 (4mn - 2m - 2n) + \frac{512}{27} (16mn + 4m + 4n), \\
 &= \frac{9824mn}{27} + \frac{496m}{9} + \frac{496n}{9}.
 \end{aligned} \tag{13}$$

(vi) The Balaban index:

The Balaban index is computed as

$$\begin{aligned}
 J(G) &= \frac{q}{q - p + 2} \sum_{ab \in E(G)} \frac{1}{\sqrt{\tilde{I}(a) \times \tilde{I}(b)}}, \\
 J(G) &= \frac{q}{q - p + 2} \left[\sum_{ab \in E_1} \frac{1}{\sqrt{\tilde{I}(a) \times \tilde{I}(b)}} + \sum_{ab \in E_2} \frac{1}{\sqrt{\tilde{I}(a) \times \tilde{I}(b)}} + \sum_{ab \in E_3} \frac{1}{\sqrt{\tilde{I}(a) \times \tilde{I}(b)}} \right], \\
 &= \frac{q}{q - p + 2} \left[\sum_{ab \in E_1} \frac{1}{\sqrt{1 \times 4}} + \sum_{ab \in E_2} \frac{1}{\sqrt{2 \times 4}} + \sum_{ab \in E_3} \frac{1}{\sqrt{4 \times 4}} \right], \\
 &= \frac{22mn}{10mn - 2} \times \left[\frac{1}{2} (12mn - 2n - 2m) + \frac{1}{2\sqrt{2}} (4mn - 2m - 2n) + \frac{1}{4} (16mn + 4m + 4n) \right].
 \end{aligned} \tag{14}$$

The numerical representation of the above-computed results is presented in Table 4.

(vii) The redefined Zagreb indices:

The redefined Zagreb indices are computed as

$$\begin{aligned}
 \text{ReG}_1(G) &= \sum_{ab \in E(G)} \frac{\tilde{I}(a) + \tilde{I}(b)}{\tilde{I}(a) \times \tilde{I}(b)}, \\
 \text{ReG}_1(G) &= \sum_{ab \in E_1} \frac{\tilde{I}(a) + \tilde{I}(b)}{\tilde{I}(a) \times \tilde{I}(b)} + \sum_{ab \in E_2} \frac{\tilde{I}(a) + \tilde{I}(b)}{\tilde{I}(a) \times \tilde{I}(b)} + \sum_{ab \in E_3} \frac{\tilde{I}(a) + \tilde{I}(b)}{\tilde{I}(a) \times \tilde{I}(b)}, \\
 &= \sum_{ab \in E_1} \frac{1+4}{1 \times 4} + \sum_{ab \in E_2} \frac{2+4}{2 \times 4} + \sum_{ab \in E_3} \frac{4+4}{4 \times 4}, \\
 &= \frac{5}{4} (12mn - 2n - 2m) + \frac{3}{4} (4mn - 2m - 2n) + \frac{1}{2} (16mn + 4m + 4n), \\
 \text{ReG}_2(G) &= \sum_{ab \in E(G)} \frac{\tilde{I}(a) + \tilde{I}(b)}{\tilde{I}(a) \times \tilde{I}(b)}, \\
 \text{ReG}_2(G) &= \sum_{ab \in E_1} \frac{\tilde{I}(a) + \tilde{I}(b)}{\tilde{I}(a) \times \tilde{I}(b)} + \sum_{ab \in E_2} \frac{\tilde{I}(a) + \tilde{I}(b)}{\tilde{I}(a) \times \tilde{I}(b)} + \sum_{ab \in E_3} \frac{\tilde{I}(a) + \tilde{I}(b)}{\tilde{I}(a) \times \tilde{I}(b)}, \\
 &= \sum_{ab \in E_1} \frac{1 \times 4}{1 + 4} + \sum_{ab \in E_2} \frac{2 \times 4}{2 + 4} + \sum_{ab \in E_3} \frac{4 \times 4}{4 + 4}, \\
 &= \frac{4}{5} (12mn - 2n - 2m) + \frac{4}{3} (4mn - 2m - 2n) + (2)(16mn + 4m + 4n), \\
 \text{ReG}_3(G) &= \sum_{ab \in E(G)} [\tilde{I}(a)\tilde{I}(b)(\tilde{I}(a) + \tilde{I}(b))], \\
 \text{ReG}_3(G) &= \sum_{ab \in E_1} [\tilde{I}(a)\tilde{I}(b)(\tilde{I}(a) + \tilde{I}(b))] \\
 &\quad + \sum_{ab \in E_2} [\tilde{I}(a)\tilde{I}(b)(\tilde{I}(a) + \tilde{I}(b))] + \sum_{ab \in E_3} [\tilde{I}(a)\tilde{I}(b)(\tilde{I}(a) + \tilde{I}(b))], \\
 &= 20(12mn - 2n - 2m) + 48(4mn - 2m - 2n) + 128(16mn + 4m + 4n), \\
 &= 2480mn + 376m + 376n.
 \end{aligned} \tag{15}$$

The numerical representation of the above computed results is presented in Table 5.

4. Heat of Formation and Entropy of Terbium IV Oxide

The topological indices $HM(G)$, $PM(G)$, $PM2(G)$, $F(G)$, $AZI(G)$, $J(G)$, $ReG1(G)$, $ReG2(G)$, and $ReG3(G)$ were calculated for various numbers of unit cells of terbium IV oxide. The thermodynamic properties of terbium IV oxide, such as heat of formation or enthalpy and entropy, are related to these indices $HM(G)$, $PM(G)$, $PM2(G)$, $F(G)$, $AZI(G)$, $J(G)$, $ReG1(G)$, $ReG2(G)$, and $ReG3(G)$. Terbium

IV oxide has a standard molar enthalpy of $-972.2 \text{ kJmol}^{-1}$, and the standard molar enthalpy for one formula unit was calculated by dividing it by Avogadro's number. The enthalpy of a cell was determined by multiplying the acquired value by the number of formula units within the cell. The enthalpy of terbium IV oxide is directly proportional to its crystal size and increases as the number of unit cells increases, according to these findings. The entropy of terbium IV oxide was calculated using the same process. The molar standard entropy of terbium IV oxide is $86.9 \text{ Jmol}^{-1}\text{K}^{-1}$. The result was then determined by multiplying the number of formula units in a single unit cell. If the number of cells gets exponential, the entropy value decreases. The downward

TABLE 4: Comparison of indices for $F(G)$, $AZI(G)$, $J(G)$ TbO_2 .

$[m, n]$	$F(G)$	$AZI(G)$	$J(G)$
[1, 1]	904	474.07	27.5
[2, 2]	3400	1675.85	99.18
[3, 3]	7488	3605.33	221.59
[4, 4]	13168	6262.52	394.26
[5, 5]	20440	9647.41	617.16
[6, 6]	29304	13760	890.28
[7, 7]	39760	18600.3	1213.63

TABLE 5: Comparison of $ReG_1(G)$, $ReG_2(G)$, $ReG_3(G)$ indices for TbO_2 .

$[m, n]$	$ReG_1(G)$	$ReG_2(G)$	$ReG_3(G)$
[1, 1]	22	54.4	3232
[2, 2]	96	202.67	11424
[3, 3]	222	444.8	24576
[4, 4]	400	780.8	42688
[5, 5]	630	1210.67	65760
[6, 6]	912	1734.4	93792
[7, 7]	1246	2352	126784

trend is the complete opposite of the heat of formation. The graphical representation is depicted in Figures 3–5.

The values for entropy and heat of formation of terbium oxide (TbO_2) for $1 \leq m \leq 7$ and $1 \leq n \leq 7$ corresponding to different formula units are computed in Table 6.

5. A Mathematical Description of Heat of Formation and Entropy of Terbium Oxide in Terms of Topological Indices

Computational approaches integrated with other disciplines of science provide a coherent way to understand a scientific problem more intensely. Usually, it is not apprehending to understand a problem based on just one science discipline, so adding some computational approaches to the study might provide a clear picture which helps to investigate the underlying phenomenon more deeply and clearly. Developing a mathematical model to describe the dynamics of objects or components involved in a study provides a very convenient mode to tackle and analyze the matter of concern. At present, software technology is playing a vital role in conducting such studies, as they provide more efficient programs to convert an experimental study into a mathematical problem and analyze it.

In this section, we have developed mathematical models to represent the thermodynamic properties, namely, heat of formation and entropy, in the form of topological indices of terbium oxide. This might provide us an efficient way to understand the molecular structure of terbium oxide based on its chemical graph structure properties. We have used the software of MATLAB to estimate such models. There are several built-in methods to fit curves between two variables. We tried all of them and found the rational method as the most efficient one as it was providing the least residuals

between empirical and fitted values. Tables 7 and 8 contain root mean squared error (RMSE), sum of squared error (SSE), and R^2 , where $ratij$ represents rational fit with numerator degree i and denominator degree j .

5.1. General Models for Indices vs. Heat of Formation. In this section, a mathematical framework has been developed between each topological index and heat of formation (HoF) of terbium oxide. All the fitted curves are shown in Figures 6–12, whereas the estimated parametric values are provided in Tables 9–15.

$$HoF(HM) = \frac{p_1}{(HM)^3 + q_1 \times (HM)^2 + q_2 \times HM + q_3}. \quad (16)$$

$$HoF(F) = \frac{p_1 \times F^2 + p_2 \times F + p_3}{F^3 + q_1 \times F^2 + q_2 \times F + q_3}. \quad (17)$$

$$HoF(AZI) = \frac{p_1 \times (AZI)^2 + p_2 \times AZI + p_3}{(AZI)^3 + q_1 \times (AZI)^2 + q_2 \times AZI + q_3}. \quad (18)$$

$$HoF(J) = \frac{p_1 \times J^2 + p_2 \times J + p_3}{J^3 + q_1 \times J^2 + q_2 \times J + q_3}. \quad (19)$$

$$HoF(ReG_1) = \frac{p_1 \times ReG_1 + p_2}{(ReG_1)^3 + q_1 \times (ReG_1)^2 + q_2 \times ReG_1 + q_3}. \quad (20)$$

FIGURE 3: $HM(G)$, $PM_1(G)$, $PM_2(G)$ indices vs. unit cell. FIGURE 4: Comparison of indices $F(G)$, $AZI(G)$, and $J(G)$ for TbO_2 .

$$HoF(ReG_2) = \frac{p_1}{(ReG_2)^3 + q_1 \times (ReG_2)^2 + q_2 \times ReG_2 + q_3} \quad (21)$$

$$HoF(ReG_3) = \frac{p_1}{(ReG_3)^3 + q_1 \times (ReG_3)^2 + q_2 \times ReG_3 + q_3} \quad (22)$$

Coefficients (with 95% confidence interval (CI)) are given in Table 9.

Coefficients (with 95% confidence bounds) are given in Table 10.

Coefficients (with 95% confidence bounds) are given in Table 11.

Coefficients (with 95% confidence bounds) are given in Table 12.

Coefficients (with 95% confidence bounds) are given in Table 13.

FIGURE 5: Comparison of $\text{ReG}_1(G)$, $\text{ReG}_2(G)$, and $\text{ReG}_3(G)$ indices for TbO_2 .TABLE 6: Values of heat of formation and entropy for different formula units of TbO_2 .

$[m, n]$	Formula units	Heat of formation $\times 10^{-21}$ kJ	Entropy $\times 10^{-22}$ kJ
[1, 1]	4	-6.456	5.768
[2, 2]	16	-0.258	0.2307
[3, 3]	32	-0.516	0.5191
[4, 4]	64	-0.0103	0.9228
[5, 5]	100	-0.0614	0.0144
[6, 6]	144	-0.0232	0.0207
[7, 7]	196	-0.0316	0.0286

TABLE 7: Goodness of fit for heat of formation vs. indices for TbO_2 .

Index	Fit type	SSE	R^2	RMSE
HM(G)	rat03	0.0121	0.9996	0.0635
F(G)	rat23	0.003584	0.9999	0.05987
AZI(G)	rat23	0.0001696	1.000	0.01302
J(G)	rat23	0.001481	1.000	0.03849
$\text{ReG}_1(G)$	rat13	0.003094	0.9999	0.03933
$\text{ReG}_2(G)$	rat03	0.005014	0.9999	0.04088
$\text{ReG}_3(G)$	rat03	0.01194	0.9997	0.06308

TABLE 8: Goodness of fit for entropy vs. indices for TbO_2 .

Index	Fit type	SSE	R^2	RMSE
HM(G)	rat13	0.001071	1.000	0.02314
F(G)	rat13	0.001065	1.000	0.02307
AZI(G)	rat03	0.001078	1.000	0.01895
J(G)	rat05	0.001031	1.000	0.0321
$\text{ReG}_1(G)$	rat14	0.001118	1.000	0.03344
$\text{ReG}_2(G)$	rat05	0.0004906	1.000	0.02215
$\text{ReG}_3(G)$	rat13	0.001069	1.000	0.02312

FIGURE 6: HoF(HM).

FIGURE 7: HoF(F).

FIGURE 8: HoF(AZI).

FIGURE 9: HoF(J).

FIGURE 10: HoF(ReG₁). FIGURE 11: HoF(ReG₂). FIGURE 12: HoF(ReG₃).

Coefficients (with 95% confidence bounds) are given in Table 15.

5.2. *General Models for Indices vs. Entropy.* This section establishes a mathematical framework between each

topological index and entropy of terbium oxide. All the fitted curves are shown in Figures 13–19 while the estimated parametric values are given in Tables 16–22.

$$\text{Entropy}(\text{HM}) = \frac{p_1 \times \text{HM} + p_2}{(\text{HM})^3 + q_1 \times (\text{HM})^2 + q_2 \times \text{HM} + q_3}. \quad (23)$$

$$\text{Entropy}(F) = \frac{p_1 \times F + p_2}{F^3 + q_1 \times F^2 + q_2 \times F + q_3}. \quad (24)$$

TABLE 9: HoF vs. HM.

	p_i	CI	q_i	CI
$i = 1$	178.2	(-9.679 e + 06, 9.679 e + 06)	1.176 e + 04	(-6.386 e + 08, 6.386 e + 08)
$i = 2$	—	—	1.94 e + 04	(-1.053 e + 09, 1.053 e + 09)
$i = 3$	—	—	7138	(-3.876 e + 08, 3.876 e + 08)

TABLE 10: HoF vs. F.

	p_i	CI	q_i	CI
$i = 1$	2.805	(-6.115 e + 05, 6.115 e + 05)	688.5	(-1.482 e + 08, 1.482 e + 08)
$i = 2$	-20.61	(-4.445 e + 06, 4.445 e + 06)	1156	(-2.493 e + 08, 2.493 e + 08)
$i = 3$	-9.782	(-2.11 e + 06, 2.11 e + 06)	444.4	(-9.587 e + 07, 9.587 e + 07)

TABLE 11: HoF vs. AZI.

	p_i	CI	q_i	CI
$i = 1$	-0.05294	(-0.3091, 0.2032)	1.691	(-1.61, 4.992)
$i = 2$	-0.03912	(-0.4201, 0.3419)	0.6454	(-4.759, 6.05)
$i = 3$	-0.005199	(-0.08769, 0.07729)	-0.008204	(-1.979, 1.962)

TABLE 12: HoF vs. J.

	p_i	CI	q_i	CI
$i = 1$	-190.1	(-1.44 e + 08, 1.44 e + 08)	1.333 e + 04	(-1.009 e + 10, 1.009 e + 10)
$i = 2$	-630	(-4.771 e + 08, 4.771 e + 08)	2.228 e + 04	(-1.687 e + 10, 1.687 e + 10)
$i = 3$	-236.6	(-1.792 e + 08, 1.792 e + 08)	8555	(-6.479 e + 09, 6.479 e + 09)

TABLE 13: HoF vs. $\text{Re}G_1$

	p_i	CI	q_i	CI
$i = 1$	-175.5	(-2.397 e + 06, 2.396 e + 06)	3781	(-5.159 e + 07, 5.16 e + 07)
$i = 2$	-112.8	(-1.541 e + 06, 1.54 e + 06)	6438	(-8.788 e + 07, 8.79 e + 07)
$i = 3$	—	—	2553	(-3.485 e + 07, 3.486 e + 07)

TABLE 14: HoF vs. $\text{Re}G_2$.

	p_i	CI	q_i	CI
$i = 1$	-0.003307	(-0.02053, 0.01391)	2.406	(1.359, 3.452)
$i = 2$	—	—	1.881	(0.1678, 3.595)
$i = 3$	—	—	0.4865	(-0.1403, 1.113)

TABLE 15: HoF vs. $\text{Re}G_3$.

	p_i	CI	q_i	CI
$i = 1$	172.1	(-9.52 e + 06, 9.52 e + 06)	1.171 e + 04	(-6.476 e + 08, 6.476 e + 08)
$i = 2$	—	—	1.93 e + 04	(-1.067 e + 09, 1.067 e + 09)
$i = 3$	—	—	7118	(-3.937 e + 08, 3.937 e + 08)

FIGURE 13: Entropy (HM).

FIGURE 14: Entropy (*F*).

FIGURE 15: Entropy (AZI).

FIGURE 16: Entropy (*J*).

FIGURE 17: Entropy (ReG_1). FIGURE 18: Entropy ReG_2 . FIGURE 19: Entropy ReG_3 .

$$\text{Entropy (AZI)} = \frac{p_1}{(\text{AZI})^3 + q_1 \times (\text{AZI})^2 + q_2 \times \text{AZI} + q_3}, \quad (25)$$

$$\text{Entropy (J)} = \frac{p_1}{J^5 + q_1 \times J^4 + q_2 \times J^3 + q_3 \times J^2 + q_4 \times J + q_5}. \quad (26)$$

TABLE 16: Entropy vs. HM.

	p_i	CI	q_i	CI
$i = 1$	0.001132	(-0.04439, 0.04666)	1.842	(1.762, 1.922)
$i = 2$	0.01288	(-0.03159, 0.05736)	0.9484	(0.8749, 1.022)
$i = 3$	—	—	0.1427	(0.1092, 0.1761)

TABLE 17: Entropy vs. F .

	p_i	CI	q_i	CI
$i = 1$	0.001791	(-0.04354, 0.04713)	1.845	(1.766, 1.925)
$i = 2$	0.01254	(-0.03159, 0.05667)	0.9604	(0.8889, 1.032)
$i = 3$	—	—	0.1465	(0.1139, 0.1792)

TABLE 18: Entropy vs. AZI.

	p_i	CI	q_i	CI
$i = 1$	0.01144	(0.007304, 0.01558)	1.845	(1.812, 1.877)
$i = 2$	—	—	0.9537	(0.9148, 0.9925)
$i = 3$	—	—	0.1431	(0.1392, 0.147)

TABLE 19: Entropy vs. J .

	p_i	CI	q_i	CI
$i = 1$	-110.9	(-2.497 e + 07, 2.497 e + 07)	2563	(-5.765 e + 08, 5.765 e + 08)
$i = 2$	—	—	-3952	(-8.901 e + 08, 8.901 e + 08)
$i = 3$	—	—	-1.355 e + 04	(-3.052 e + 09, 3.052 e + 09)
$i = 4$	—	—	-8056	(-1.814 e + 09, 1.814 e + 09)
$i = 5$	—	—	-1311	(-2.951 e + 08, 2.951 e + 08)

TABLE 20: Entropy vs. ReG_1 .

	p_i	CI	q_i	CI
$i = 1$	1.041	(-1.206 e + 06, 1.206 e + 06)	-1145	(-1.341 e + 09, 1.341 e + 09)
$i = 2$	-10.05	(-1.175 e + 07, 1.175 e + 07)	-2126	(-2.487 e + 09, 2.487 e + 09)
$i = 3$	—	—	-1121	(-1.311 e + 09, 1.311 e + 09)
$i = 4$	—	—	-170.7	(-1.996 e + 08, 1.996 e + 08)

TABLE 21: Entropy vs. ReG_2 .

	p_i	CI	q_i	CI
$i = 1$	103.9	(-2.399 e + 06, 2.399 e + 06)	-3508	(-8.104 e + 07, 8.103 e + 07)
$i = 2$	—	—	-384.3	(-8.831 e + 06, 8.83 e + 06)
$i = 3$	—	—	7836	(-1.81 e + 08, 1.81 e + 08)
$i = 4$	—	—	5312	(-1.227 e + 08, 1.227 e + 08)
$i = 5$	—	—	909.8	(-2.101 e + 07, 2.101 e + 07)

TABLE 22: Entropy vs. ReG_3 .

	p_i	CI	q_i	CI
$i = 1$	0.001368	(-0.04409, 0.04682)	1.843	(1.763, 1.923)
$i = 2$	0.01276	(-0.0316, 0.05712)	0.9527	(0.8799, 1.025)
$i = 3$	—	—	0.144	(0.1109, 0.1772)

$$\text{Entropy}(\text{ReG}_1) = \frac{p_1 \times \text{ReG}_1 + p_2}{(\text{ReG}_1)^4 + q_1 \times (\text{ReG}_1)^3 + q_2 \times (\text{ReG}_1)^2 + q_3 \times \text{ReG}_1 + q_4}. \quad (27)$$

$$\text{Entropy}(\text{ReG}_2) = \frac{p_1}{(\text{ReG}_2)^5 + q_1 \times (\text{ReG}_2)^4 + q_2 \times (\text{ReG}_2)^3 + q_3 \times (\text{ReG}_2)^2 + q_4 \times \text{ReG}_2 + q_5}. \quad (28)$$

$$\text{Entropy}(\text{ReG}_3) = \frac{p_1 \times \text{ReG}_3 + p_2}{(\text{ReG}_3)^3 + q_1 \times (\text{ReG}_3)^2 + q_2 \times \text{ReG}_3 + q_3}. \quad (29)$$

Coefficients (with 95% confidence bounds) are given in Table 16.

Coefficients (with 95% confidence bounds) are given in Table 17.

Coefficients (with 95% confidence bounds) are given in Table 18.

Coefficients (with 95% confidence bounds) are given in Table 19.

Coefficients (with 95% confidence bounds) are given in Table 20.

Coefficients (with 95% confidence bounds) are given in Table 21.

Coefficients (with 95% confidence bounds) are given in Table 22.

6. Conclusions

A connection between topological indices and thermodynamic properties of terbium IV oxide has been developed. This study helps to understand the chemical structure of terbium IV oxide based on the graphical properties of its underlying graph more deeply as this was economical and more efficient. Curve fitting techniques have been utilized to establish such a relation among indices and heat of formation and entropy. The rational fitting approach was selected based on its efficacy. This direct connection might help to explore the dynamical properties of this terbium IV oxide.

Data Availability

The data used to support the findings of this study are cited at relevant places within the text as references.

Conflicts of Interest

The authors declare no conflicts of interest.

Authors' Contributions

All authors contributed equally to this work.

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