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Original research article

On Generalized ISI Index of the Crystallographic Structure of Tin Dioxide

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ABSTRACT

Topological indices are molecular descriptors that help in understanding the physical, chemical and biological properties of molecular structures. The generalization of the Inverse Sum Indeg (ISI) index can be used to obtain many standard degree-based topological indices. In this paper, we have computed the generalized ISI index and its associated topological indices for the crystallographic structure of Tin dioxide, SnO_2. These indices are expressed in terms of three variables (l, m, n) such that each corresponds to a particular direction in the growth of the SnO_2 crystal. The variation of the topological indices with respect to the three parameters is also studied graphically.

Keywords: Crystallographic structure; ISI index; SnO_2; Topological index

1. Introduction

Graph theory plays a significant role in the study of chemical structures. This theory is used for mathematically modeling chemical structures to get an idea of the physical and chemical properties of the chemical compounds. It is also used to design complex networks. A molecular graph is represented by vertices and edges where the vertices denote atoms and the edges denote the molecular bonds between them. Chemical graph theory is a branch of mathematical chemistry that applies combinatorial and geometrical graph theory to model the structure of molecules. Chemical compounds have several applications in chemical graph theory, drug design, etc.

Topological indices (TIs) are molecular descriptors used in chemical graph theory. They are graph invariants that depict some useful information regarding the topology of a molecule. They are an important tool in mathematical chemistry, especially in the development of QSAR and QSPR studies [1-5]. They correlate the chemical structures with many physicochemical properties. The last few

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years have witnessed an increased attention among researchers towards the study of topological indices as a powerful means in the illustration of molecular structure. Besides these, TIs play a significant role in network theory, spectral graph theory, etc. Recently, some of the TIs which we are going to study were introduced for fuzzy graphs by Islam and Pal [6-8]. They also discussed various applications of these TIs defined for fuzzy graphs. The Wiener Index (WI) is the first topological index proposed by Harold Wiener [9] in 1947 and is the most widely used distance-based topological index. Wiener also proved that the boiling point of paraffins depends on WI.

Degree-based topological indices have been extensively studied as they can correlate with many properties of molecular compounds. The definitions of some of these indices which will be used in our study are given below:

Let $G=(V,E)$ be a simple connected graph, where $V(G)$ is the vertex set and $E(G)$ be the edge set of the graph G. The degree of a vertex $v\in V(G)$ is denoted by $d_G(v)$ or $d(v)$.

Gutman and Trinajstic [10] introduced the first and second Zagreb indices which are used to calculate pi- electron energy of a conjugate system. These indices are defined as follows:

- First Zagreb Index

$$M_1(G) = \sum_{v\in V(G)} d_G(v)^2 = \sum_{uv\in E(G)} [d_G(u) + d_G(v)].$$

- Second Zagreb Index

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

In 1975, Milan Randić [5] proposed the Randić index (connectivity index). The Randić index is used to measure carbon atom skeleton of saturated hydrocarbons and has many applications in chemistry and pharmacology. It is defined as

$$R(G) = \sum_{uv\in E(G)} (d(u)\, d(v))^{\frac{-1}{2}}.$$

The Sum-connectivity index was put forward by Zhou and Trinajstić [11] and is defined as

$$SCI(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u) + d(v)}}.$$

The inverse sum indeg index denoted by *ISI*(*G*) is a significant predictor of total surface area of octane isomers and is defined as [12]

$$ISI(G) = \sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u) + d(v)}.$$

Shirdel et al., in 2013 [13] defined the Hyper Zagreb index as

$$HM(G) = \sum_{uv\in E(G)} [d_G(u)+d_G(v)]^2.$$

The Harmonic index [14], *H*(*G*) is defined as

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d(u) + d(v)}.$$

The Geometric-Arithmetic index [4] of a graph G is defined as

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}.$$

Bollobás and Erdös [15] in 1998 and Amić et al. [16] independently generalized the Randić index and defined the first generalized Randić index as

$$R_{\alpha}(G) = \sum_{uv \in E(G)} (d(u)\, d(v))^{\alpha},$$

where $\alpha \neq 0, \alpha \in \mathbb{R}$. Considering, $\alpha = \frac{-1}{2}$ in the generalized Randić index we get the Randić index. In a similar manner, Zhou and Trinajstić [17] generalized the first zagreb index and the sum-connectivity index and defined the general sum-connectivity index as

$$\chi_{\alpha}(G) = \sum_{uv \in E(G)} (d(u) + d(v))^{\alpha}.$$

Tin (IV) oxide (SnO_2) is one of the most widely studied metal oxides. It has grabbed the attention of researchers for its excellent physical and chemical properties which include electrical conductivity, mechanical properties, high chemical stability, and optical transparency. The material has been extensively used in gas sensors, thin-film transistors (TFT), batteries, photovoltaic cells, fuel cells, transparent electronics, and so on [18-22]. Tin dioxide is regarded as an n-type semiconductor with a wide band gap (~3.6 eV). It is also studied as a catalyst in several organic reactions.

In the literature it has been found that TIs of various anticancer drugs [23], nanostardendrimer and V-phenylenic-nanotorous [24], 68 types of alkanes [25], saturated and unsaturated hydrocarbons [26], nanosheets, nanotubes and nanotori of SiO_2 [27], pruned quartz and its related structures [28], 2 Boron nanotubes [29], single walled TiO_2 nanotube [30], Li_n-clusters [31] have been calculated and in some of them the relation between TIs and various physico-chemical properties have also been studied. For more details, one may refer to [32]

Some recent works on the computation of topological indices of 2D and 3D crystals are listed as: Gao et al. calculated topological indices of carbon graphite and crystal cubic carbon structure in [33], crystallographic structure of molecules Cu_2O and TiF_2 using M-polynomial in [34], Yang et al. studied degree-distance based indices of crystal cubic carbon structure in [35], topological characterization of the crystallographic structures of Cu_2O and TiF_2 was done by Yang et al. in [36], M-polynomial and related indices of benzene ring are investigated by Yang et al. in [37], Chaudhury et al. studied M-polynomial and some degree-based TIs of Cu_2O crystal in [38] and Baishya et al. [32] studied the TIs of 3-D TiO_2 crystal structure using the M-polynomial.

From the literature review, it is observed that most of the computations of TIs are found for hydrocarbons and 2D systems. Only a few works have been done on 3D systems. Moreover, from the available literature it can be found that the generalized ISI index and its related indices are not computed for any crystal structure. This motivated us to work on this detail.

In this paper, we have computed the generalized ISI index and the related topological indices of crystallographic structure of SnO_2. Also, the variation of these indices with respect to the given parameters l, m, n is shown graphically. These variations can be correlated with any size dependent physical property of the SnO_2 crystal.

2. Topological Indices Derived from Generalized ISI Index

With motivation from the paper by Gutman et al. [39], a generalized degree-based topological index was recently proposed by Buragohain et al. in [40]. This new index is named generalized ISI index denoted by $\mathrm{ISI}_{(\alpha,\beta)}(G)$ and is defined as

$$ISI_{(a,b)}(G) = \sum_{uv\in E(G)} (d(u)d(v))^{a}(d(u)+d(v))^{b},$$

where α and β are some real numbers. It is seen that for $\alpha = 1$, and $\beta = -1$ this index is the ISI index.

Table1. Relationships between $ISI_{(\alpha,\beta)}(G)$ - index and some other T.I.'s.

Topological index	Notation	Corresponding $ISI_{(\alpha,\beta)}(G)$ index
First Zagreb index	$M_1(G)$	$ISI_{0,1}(G)$
Second Zagreb index	$M_2(G)$	$ISI_{1,0}(G)$
Randić index	R(G)	$ISI_{-\frac{1}{2},0}(G)$
Sum connectivity index	SCI(G)	$ISI_{0,\frac{-1}{2}}(G)$
Inverse sum indeg index	ISI(G)	$ISI_{1,-1}(G)$
Harmonic index	H(G)	$2ISI_{0,-1}(G)$
Geometric-Arithmetic Mean index	GA(G)	$2ISI_{\frac{1}{2},-1}(G)$
Hyper-Zagreb index	HM(G)	$ISI_{0,2}(G)$
First Generalized Randić index	$R_\alpha(G)$	$ISI_{\alpha,0}(G)$
General sum-connectivity index	$\chi_\alpha(G)$	$ISI_{0,\alpha}(G)$

Instead of calculating independently, we can calculate the degree-based TIs given in the literature directly from the generalized Inverse Sum Indeg (ISI) index. This may lead to better correlation with various physicochemical properties of chemical compounds and the development of the existing results. The above table (Table 1) due to Buragohain et al. [40] relates the above-defined degree-based TIs with the generalized ISI index.

3. Molecular Graph of SnO_2 Crystal

Let us consider G to be the molecular graph for the crystallographic structure of SnO_2 $[l,m,n]$ with $l \times m$ number of unit cells in the plane and n layers. The total number of vertices and edges for this graph are $(l+1)(m+1)(n+1) + 5lmn + 2ln$ and $10lmn + 2l(m+1)n + (l+1)m(n+1)$, respectively. From the molecular graph, we get $|d_2| = 8 + 4l, |d_3| = 4(l-1) + 2(m-1) + 4(n-1) + 2nl(m-1), |d_4| = 2(m-1)+, |d_5| = 2(l-1)(m-1) + (n-1)(2l+2m-4), |d_6| = lmn$ and $|d_8| = (l-1)(m-1)(n-1)$. Here $|d_i|$ denote the numbers of the i[th] -degree vertex in SnO_2 $[l,m,n]$.

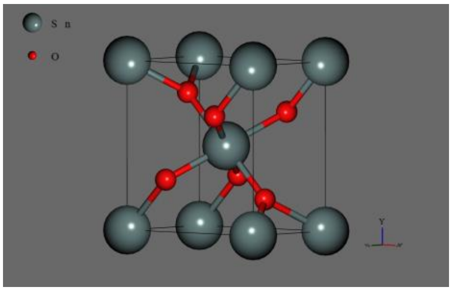

Fig. 1. Crystal structure of $SnO_2[1,1,1]$.

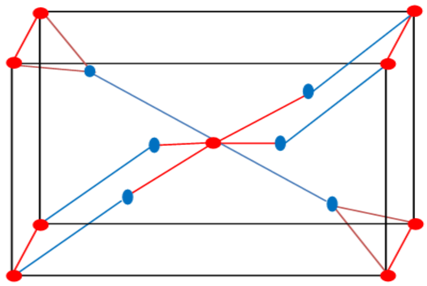

Fig. 2. Molecular graph of $SnO_2[1,1,1]$.

We observe from Fig. 1. that in the unit cell of SnO_2, the degree of the oxygen atom is 2 but the actual degree of these atoms in formation of the SnO_2 supercell is 3. The missing one degree is shared with another unit cell. As a result, for the complete understanding of degree of these oxygen atoms we need to consider the supercell. The molecular graph of crystallographic structure of SnO_2 [2, 2, 2] is shown in Fig. 3.

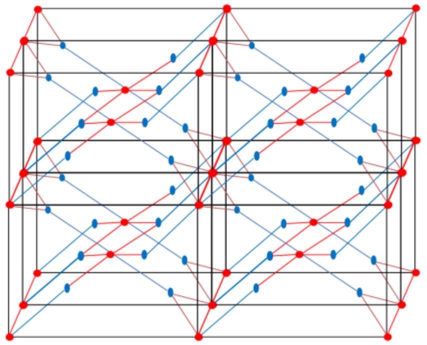

Fig. 3. Molecular graph of crystallographic structure of SnO_2 [2, 2, 2].

In this paper, the different relations such as vertices, edges and T.I. are expressed in terms of l, m, n where $l > 1,\ m > 1,\ n > 1$ and are found to be invalid for $l = m = n = 1$. This implies that these definitions are not applicable for a single unit cell.

The edge set of $SnO_2[l,m,n] \cong G[l,m,n]$ has the following fourteen partitions,

$$E_1 = \{e = uv \in E(G) \mid d_u = 2,\ d_v = 2\},$$
$$E_2 = \{e = uv \in E(G) \mid d_u = 2,\ d_v = 3\},$$
$$E_3 = \{e = uv \in E(G) \mid d_u = 2,\ d_v = 4\},$$
$$E_4 = \{e = uv \in E(G) \mid d_u = 2,\ d_v = 5\},$$
$$E_5 = \{e = uv \in E(G) \mid d_u = 2,\ d_v = 6\},$$
$$E_6 = \{e = uv \in E(G) \mid d_u = 3,\ d_v = 3\},$$
$$E_7 = \{e = uv \in E(G) \mid d_u = 3,\ d_v = 4\},$$
$$E_8 = \{e = uv \in E(G) \mid d_u = 3,\ d_v = 5\},$$
$$E_9 = \{e = uv \in E(G) \mid d_u = 3,\ d_v = 6\},$$
$$E_{10} = \{e = uv \in E(G) \mid d_u = 3,\ d_v = 8\},$$
$$E_{11} = \{e = uv \in E(G) \mid d_u = 4,\ d_v = 4\},$$
$$E_{12} = \{e = uv \in E(G) \mid d_u = 5,\ d_v = 5\},$$
$$E_{13} = \{e = uv \in E(G) \mid d_u = 5,\ d_v = 8\},$$
$$E_{14} = \{e = uv \in E(G) \mid d_u = 8,\ d_v = 8\}.$$

The cardinalities of the above-mentioned edge partitions are as given below:

$$|E_1(G)| = 4, |E_2(G)| = 4l + 4n, |E_3(G)| = 4,$$
$$|E_4(G)| = 4l \times n - 4l - 4n + 4, |E_5(G)| = 4nl,$$
$$|E_6(G)| = 4l + 2m + 4n - 10, |E_7(G)| = 4m - 4,$$

$$|E_8(G)| = 6lm + 4nl + 6mn - 6l - 12m - 6n + 8,$$
$$|E_9(G)| = 4lmn, |E_{10}(G)| = 6lmn - 6lm - 6nl$$
$$-6mn + 6l + 6m + 6n - 6, |E_{11}(G)| = 2m - 4,$$
$$|E_{12}(G)| = 2lm + 2mn - 4l - 4m - 4n + 8,$$
$$|E_{13}(G)| = 2nl - 2l - 2n + 2, |E_{14}(G)| =$$
$$lmn - lm - 2nl - mn + 2l + m + 2n - 2.$$

4. Topological Indices of SnO_2 Crystal

4.1 $ISI_{(\alpha,\beta)}$-index of SnO_2 [l, m, n]

Let us consider the graph $G(l,m,n)$ of SnO_2 with $l > 1,\ m > 1,\ n > 1$. Then, the generalized ISI index of the graph is given by

$$ISI_{(\alpha,\beta)}(G(l,m,n)) = \sum_{uv \in E(G)} (d(u)d(v))^{\alpha}(d(u) + d(v))^{\beta}$$

$$= \sum_{uv \in E_1(G(l,m,n))} (2\times 2)^{\alpha}(2 + 2)^{\beta} + \sum_{uv \in E_2(G(l,m,n))} (2\times 3)^{\alpha}(2 + 3)^{\beta}$$
$$+ \sum_{uv \in E_3(G(l,m,n))} (2\times 4)^{\alpha}(2 + 4)^{\beta} + \sum_{uv \in E_4(G(l,m,n))} (2\times 5)^{\alpha}(2 + 5)^{\beta}$$
$$+ \sum_{uv \in E_5(G(l,m,n))} (2\times 6)^{\alpha}(2 + 6)^{\beta} + \sum_{uv \in E_6(G(l,m,n))} (3\times 3)^{\alpha}(3 + 3)^{\beta}$$
$$+ \sum_{uv \in E_7(G(l,m,n))} (3\times 4)^{\alpha}(3 + 4)^{\beta} + \sum_{uv \in E_8(G(l,m,n))} (3\times 5)^{\alpha}(3 + 5)^{\beta}$$
$$+ \sum_{uv \in E_9(G(l,m,n))} (3\times 6)^{\alpha}(3 + 6)^{\beta} + \sum_{uv \in E_{10}(G(l,m,n))} (3\times 8)^{\alpha}(3 + 8)^{\beta}$$
$$+ \sum_{uv \in E_{11}(G(l,m,n))} (4\times 4)^{\alpha}(4 + 4)^{\beta} + \sum_{uv \in E_{12}(G(l,m,n))} (5\times 5)^{\alpha}(5 + 5)^{\beta}$$
$$+ \sum_{uv \in E_{13}(G(l,m,n))} (5\times 8)^{\alpha}(5 + 8)^{\beta} + \sum_{uv \in E_{14}(G(l,m,n))} (8\times 8)^{\alpha}(8 + 8)^{\beta}$$
$$= \sum_{uv \in E_1(G(l,m,n))} (4)^{\alpha}(4)^{\beta} + \sum_{uv \in E_2(G(l,m,n))} (6)^{\alpha}(5)^{\beta} + \sum_{uv \in E_3(G(l,m,n))} (8)^{\alpha}(6)^{\beta}$$
$$+ \sum_{uv \in E_4(G(l,m,n))} (10)^{\alpha}(7)^{\beta} + \sum_{uv \in E_5(G(l,m,n))} (12)^{\alpha}(8)^{\beta} + \sum_{uv \in E_6(G(l,m,n))} (9)^{\alpha}(6)^{\beta}$$
$$+ \sum_{uv \in E_7(G(l,m,n))} (12)^{\alpha}(7)^{\beta} + \sum_{uv \in E_8(G(l,m,n))} (15)^{\alpha}(8)^{\beta} + \sum_{uv \in E_9(G(l,m,n))} (18)^{\alpha}(9)^{\beta}$$

$$+\sum_{uv\in E_{10}(G(l,m,n))}(24)^{\alpha}(11)^{\beta}+\sum_{uv\in E_{11}(G(l,m,n))}(16)^{\alpha}(8)^{\beta}+\sum_{uv\in E_{12}(G(l,m,n))}(25)^{\alpha}(10)^{\beta}$$
$$+\sum_{uv\in E_{13}(G(l,m,n))}(40)^{\alpha}(13)^{\beta}+\sum_{uv\in E_{14}(G(l,m,n))}(64)^{\alpha}(16)^{\beta}$$
$$= |E_1(G(l,m,n))|(4)^{\alpha}(4)^{\beta}+|E_2(G(l,m,n))|(6)^{\alpha}(5)^{\beta}$$
$$+|E_3(G(l,m,n))|(8)^{\alpha}(6)^{\beta}+|E_4(G(l,m,n))|(10)^{\alpha}(7)^{\beta}$$
$$+|E_5(G(l,m,n))|(12)^{\alpha}(8)^{\beta}+|E_6(G(l,m,n))|(9)^{\alpha}(6)^{\beta}$$
$$+|E_7(G(l,m,n))|(12)^{\alpha}(7)^{\beta}+|E_8(G(l,m,n))|(15)^{\alpha}(8)^{\beta}$$
$$+|E_9(G(l,m,n))|(18)^{\alpha}(9)^{\beta}+|E_{10}(G(l,m,n))|(24)^{\alpha}(11)^{\beta}$$
$$+|E_{11}(G(l,m,n))|(16)^{\alpha}(8)^{\beta}+|E_{12}(G(l,m,n))|(25)^{\alpha}(10)^{\beta}$$
$$+|E_{13}(G(l,m,n))|(40)^{\alpha}(13)^{\beta}+|E_{14}(G(l,m,n))|(64)^{\alpha}(16)^{\beta}$$
$$=(4)^{a+b+1}+(4l+4n)(6)^{a}(5)^{b}+(2)^{3a+b+2}(3)^{b}$$
$$+(4\ln-4n+4)(10)^{a}(7)^{b}+(4\ln)(3)^{a}(2)^{2a+3b}$$
$$+(4l+2m+4n-10)(3)^{2a+b}(2)^{b}+(4m-4)(12)^{a}(7)^{b}$$
$$+(6lm+4\ln+6mn-6l-12m-6n+8)(15)^{a}(8)^{a}$$
$$+(4lmn)(2)^{a}(3)^{2a+2b}+(6lmn-6lm-6\ln-6mn$$
$$+(2lm+2mn-4l-4m-4n+8)(5)^{2a+b}(2)^{b}$$
$$+(2\ln-2l-2n+2)(40)^{a}(13)^{b}+(lmn-lm-2\ln-mn$$
$$+2l+m+2n-2)(64)^{a}(16)^{b}.$$

4.2 Computation of Topological indices from generalized ISI index

Consider the graph of $G\cong SnO_2[l,m,n]$ with $l,\ m,\ n>1.$ Then the above defined degree-based topological indices are computed from generalized ISI index as:

1) $M_1(G)\ =\ 118lmn-14lm+20\ln-14mn+2m+20.$

2) $M_2(G)\ =\ 280lmn-68lm-44\ln-68mn+22l$ $+\ 26m+22n+14.$

3)
$$R(G)=2+\frac{4}{\sqrt{6}}(l+n)+\sqrt{2}+\frac{4}{\sqrt{10}}(\ln-l-n+1)+\frac{2}{\sqrt{3}}\ln$$
$$+\frac{2}{3}(2l+m+2n-5)+\frac{4}{\sqrt{12}}(m-1)$$
$$+\frac{2}{\sqrt{15}}(3lm+2\ln+3mn-3l-6m-3n4)$$
$$+\frac{4}{3\sqrt{2}}lmn+\frac{6}{\sqrt{24}}(lmn-lm-\ln-mn+l+m+n-1)$$
$$+\frac{2}{\sqrt{16}}(m-2)+\frac{2}{5}(lm+mn-2l-2m-2n+4)+\frac{2}{\sqrt{40}}(\ln-l-n+1)$$
$$+\frac{1}{\sqrt{64}}(lmn-lm-2\ln-mn+2l+2n+m-2).$$

4)
$$SCI(G)=2+\frac{4}{\sqrt{5}}(l+n)+\frac{\sqrt[3]{2}}{\sqrt{3}}+\frac{4}{\sqrt{7}}(\ln-l-n+1)$$
$$+\frac{4}{\sqrt[3]{2}}\ln+\frac{2}{\sqrt{6}}(2l+m+2n-5)+\frac{4}{\sqrt{7}}(m-1)$$
$$+\frac{2}{\sqrt{8}}(3lm+2\ln+3lmn-3l-6m-3n+4)+\frac{4}{3}lmn$$
$$+\frac{6}{\sqrt{11}}(lmn-lm-\ln-mn+l+m+n-1)+\frac{2}{\sqrt{8}}(m-2)$$
$$+\frac{2}{\sqrt{10}}(lm+mn-2l-2m-2n+4)+\frac{2}{\sqrt{13}}(\ln-l-n+1)$$
$$+\frac{1}{\sqrt{15}}(lmn-lm-2\ln-mn+2l+2n+m-2).$$

5)
$$ISI(G)=4+\frac{24}{5}(l+n)+\frac{16}{3}+\frac{40}{7}(\ln-l-n+1)$$
$$+6\ln+\frac{1}{3}(2l+m+2n-5)+\frac{48}{7}(m-1)$$
$$+\frac{15}{4}(3lm+2\ln+3mn-3l-6m-3n+4)$$
$$+8lmn+\frac{144}{11}(lmn-lm-\ln-mn+l+m+n-1)$$
$$+4(m-2)+5(lm+mn-2l-2m-2n+4)$$
$$+\frac{80}{13}(\ln-l-n+1)+4(lmn-lm-2\ln-mn+2l$$
$$+2n+m-2).$$

6)
$$H(G)=2+\frac{8}{5}(l+n)+\frac{4}{3}+\frac{8}{7}(\ln-l-n+1)$$
$$+\ln+\frac{2}{3}(2l+m+2n-5)+\frac{8}{7}(m-1)$$
$$+\frac{1}{2}(3lm+2\ln+3mn-3l-6m-3n+4)+\frac{8}{9}lmn$$
$$+\frac{12}{11}(lmn-lm-\ln-mn+l+m+n-1)+\frac{1}{2}(m-2)$$
$$+\frac{4}{10}(lm+mn-2l-2m-2n+4)+\frac{4}{13}(\ln-l-n+1)$$
$$+\frac{2}{16}(lmn-lm-2\ln-mn+2l+2n+m-2).$$

7)

$$GA(G)=2+\frac{8\sqrt{6}}{5}(l+n)+\frac{\sqrt[7]{2}}{3}+\frac{8\sqrt{10}}{7}(ln-l$$
$$-n+1)+2\sqrt{3}\,ln+2(2l+m+2n-5)$$
$$+\frac{8\sqrt{12}}{7}(m-1)+\frac{\sqrt{15}}{2}(3lm+2ln+3mn-3l-6m$$
$$-3n+4)+\frac{8\sqrt{2}}{3}lmn+\frac{6\sqrt{24}}{11}(lmn-lmn-ln$$
$$-mn+l+m+n-1)+\frac{\sqrt{16}}{4}(m-2)+2(lm+mn$$
$$-2l-2m-2n+4)+\frac{4\sqrt{40}}{13}(nl-l-n+1)$$
$$+\frac{\sqrt{64}}{16}(lmn-lm-2ln-mn+2l+2n+m-2).$$

8) $HM(G)=1306lmn-398lm-192ln$
$-398mn+164l+210m+164n+4.$

9)

$$R_\alpha(G)=2^\alpha\cdot2^\alpha\cdot4+2^\alpha\cdot3^\alpha\cdot4(l+n)+2^\alpha$$
$$\cdot4^\alpha\cdot4+2^\alpha\cdot5^\alpha\cdot4(l-1)(n-1)+2^\alpha\cdot6^\alpha$$
$$\cdot4ln+3^\alpha\cdot3^\alpha\cdot2\cdot(2l+m+2n\text{-}5)+3^\alpha\cdot4^\alpha$$
$$\cdot4(m-1)+3^\alpha\cdot5^\alpha\cdot2(3lm+2ln+3mn-3l$$
$$-6m-3n+4)+3^\alpha\cdot6^\alpha\cdot4lmn+3^\alpha\cdot8^\alpha$$
$$\cdot6(lmn-lm-ln-mn+l+m+n-1)+4^\alpha$$
$$\cdot4^\alpha\cdot2(m-2)+5^\alpha\cdot5^\alpha\cdot2(lm+mn-2l-2m$$
$$-2n+4)+5^\alpha\cdot8^\alpha\cdot2(l-1)(n-1)+8^\alpha\cdot8^\alpha(lmn$$
$$-lm-2ln-mn+2l+2n+m-2).$$

10)

$$\chi_\alpha(G)=2^\alpha\cdot2^\alpha\cdot4+5^\alpha\cdot4(l+n)+2^{\alpha+2}$$
$$\cdot3^\alpha+7^\alpha\cdot4(l-1)(n-1)+2^{3\alpha}\cdot4ln+3^\alpha\cdot2^\alpha$$
$$\cdot2(2l+m+2n-5)+7^\alpha\cdot4(m-1)+8^\alpha\cdot2(3lm$$
$$+2ln+3mn-3l-6m-3n+4)+3^{2\alpha}\cdot4lmn$$
$$+11^\alpha\cdot6(lmn-lm-ln-mn+l+m+n-1)$$
$$+8^\alpha\cdot2(m-2)+5^\alpha\cdot2^\alpha\cdot2(lm+mn-2l-2n+4)$$
$$+13^\alpha\cdot2(l-1)(n-1)+16^\alpha\cdot(lmn-lm-2ln-mn$$
$$+2l+2n+m-2).$$

5. Plots of topological indices

In Figs. 4-6, the variation of different topological indices with respect to the parameters l, m, n is shown respectively. It is seen that all the variations are linear having different slopes.

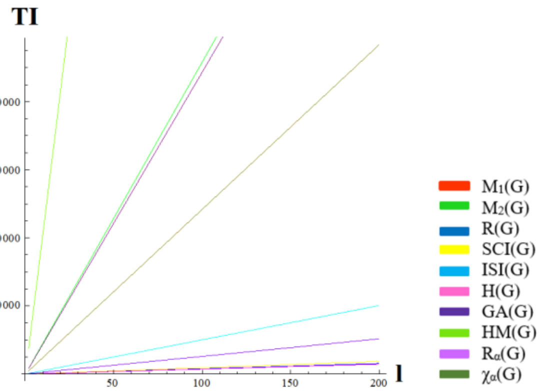

Fig. 4. Plot of different TIs vs *l*.

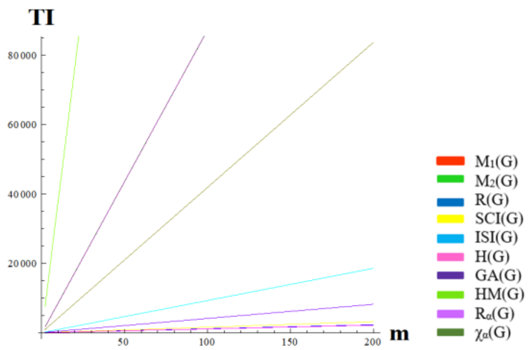

Fig. 5. Plot of different TIs vs *m*.

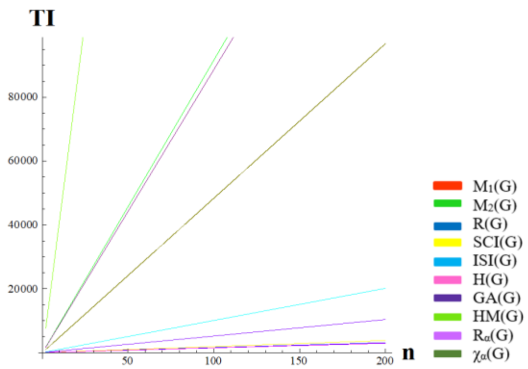

Fig. 6. Plot of different TIs vs *n*.

The slope of $HM(G)$ is highest in all three cases. All the topological indices maintain almost the same order of slopes in all the plots but with an exception of $M_2(G)$ in Fig. 5. The slope of the plot of $M_2(G)$ vs m decreases (Fig. 5) as compared to that vs l and n (Figs. 4 and 6), respectively. This kind of variation can be helpful in the study of various physicochemical properties of the chemical compounds.

5. Conclusions

The generalized Inverse Sum Indeg (ISI) index is interesting because it helps to compute many standard degree-based topological indices. We have computed the generalized ISI index and its related degree-based topological indices for the crystallographic structure of SnO_2. Also, we presented graphical representation of the topological indices along the parameters (l,m,n). Topological indices calculated in this manner help us to predict many physical, chemical and biological properties of the understudy molecular compound. The results obtained can play a vital role in the study of SnO_2 and its applications by reducing the time needed to calculate each topological descriptor one by one. In the future, we are keen to study some new chemical compounds and compute the index.

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