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On certain degree based Zagreb and Randić indices for cubic tungsten trioxide $[p,q,r]$ nanomultilayer

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Abstract

Topological index is one of the significant tools in chemical graph theory, and is designed to transform a molecular map into a number. Basically, topological index is a single numeric quantity which characterises the entire chemical structure of a compound. Topological indices are crucial relevance to the physicochemical properties of the molecular compounds and also predicting their bioactivity. As an n-type semiconducting metal oxide, cubic tungsten trioxide (hereafter $c-WO_3$) nanostructure has been considered as a potential candidate, which offers manifold applications. Therefore, the chemistry of $c-WO_3$ is very important and its interdisciplinary study provides a way to understand the importance of various domains. In this study, we computed certain degree based Zagreb and Randić topological indices for $c-WO_3$ nanomultilayer for all values of p,q and r by adopting edge partition technique. The computational results are analysed, compared and the general formulas to the indices are obtained.

Keywords

Topological index, Zagreb, Randić, WO_3 nanomultilayer, Molecular graph.

AMS Subject Classification

05C05, 05C12, 05C50.

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Contents

1. Introduction

Chemical compounds are often modelled by molecular graphs. Mathematical chemistry has a lot of potential tools in real life such as topological indices, which are served as molecular descriptors to reveal the unknown facts behind the symmetry of molecular graphs. Topological index is a graph-theoretical invariant, which provides a mathematical formulation to chemical structures through their molecular graphs and also describes their topology [1-3]. Owing to its mathematical nature in chemical graph theory this idea has drawn the attention of many researchers. Topological indices are being widely employed to correlate and predict certain physicochemical properties (e.g. solubility [4] and refractive index [5]) and thermodynamic properties (eg. vaporization [6] and heats of formation [7]) of molecular species without using quantum mechanics. To get more information about topological indices and their significance, we should refer the following texts [8-10] to the reader.

Let $G=(V,E)$ be a (molecular) graph with vertex set V and edge set E. Edge of G is represented by $e=uv$, connecting the vertices u and v. For each vertex v of G, the degree of v is denoted by d_v and is defined as number of vertices adjacent to v. Suppose Ω denotes the class of all graphs, then a function $\Psi:\Omega\to R^+$ is said to be a topological index if $A\cong B$ implies $\Psi(A)=\Psi(B)$. Throughout this article only simple connected graphs (i.e. connected graphs without self loops and parallel edges) are considered. For more related on algebraic and graph theoretical tools used herein, the reader is referred to the following text [11].

To date, numerous topological descriptors were established

such as distance based, degree based, eccentricity based and spectral based topological indices. Topological indices were first introduced by Wiener for predicting certain physical properties of alkanes in 1947 [12]. In 1972, Gutman and Trinajstic have been derived a pair of degree based topological indices named as the first Zagreb index $M_l(G)$ and second Zagreb index $M_2(G)$, which are employed as branching indices and are used in the development of structure property modelling, QSAR (quantitative structure-activity relationship) and QSPR (quantitative structure-property relationship) studies [13]. These indices were helpful in the topological formula for predicting the total $\pi-$ electron energy of conjugated molecules [14]. Later, third Zagreb index was brought into light by Fath-Tabar et al. [15]. In this line, hyper Zagreb indices [16], Reduced second Zagreb index [17], Redefined Zagreb indices [18], Nano-Zagreb index [19] and Sum Nano-Zagreb index [20] were introduced and discussed by respective authors in their research articles. In 1975, Milan Randić introduced a connectivity index known as branching index (later called as Randić index) which is represented by $\chi(G)$ and served as a reliable tool for quantitative assessment of branching of molecules, QSAR and QSPR studies [6]. Many modified forms of Randić indices were established such as, general Randić index [21], Reciprocal Randić index [22], Reduced Reciprocal Randić index, [23], modified Randić index [24] and Zeroth$-$ order general Randić index $[25-28]$ and so on.

The interdisciplinary co-operation among various domains such as chemical graph theory, materials science and computational methods paving a way of new dimension in the development of nanotechnology. For instance, Idrees et al. [29] have proposed the topological Indices for H-Naphtalenic nanosheet. Bača et al. [30] computed the topological indices for the carbon nanotube networks. Afzal et al. [31] have demonstrated some topological indices of OT $[m,n]$ Octagonal Tillings and TiO_2 nanotubes. Javaid et al. [32] have reported certain topological indices of Titania Nanotube $TiO_2[m,n]$. Munir et al. [33] have discussed certain computational aspects of triangular Boron nanotubes. Topological Indices of the Pent- Heptagonal Nanosheets VC_5C_7 and HC_5C_7 were discussed by Deng et al. in [34].

In this scenario, we compute and analyse various Zagreb and Randić topological indices for $c-WO_3[p,q,r]$ nanomultilayer through its molecular graph, which is precisely the contribution of this study. To the best of our knowledge, Zagreb and Randić topological indices of WO_3 nanomultilayer have not been reported yet. It is worth mentioning that, WO_3 is one of the most investigated nanomaterials due to its unique physicochemical properties such as high surface area to volume ratios, various surface morphologies, wider optical band gap and tunable transport properties, which are very benefices in gas sensing devices, water splitting applications and photocatalytic activities [35]. Details about the applications of WO_3 nanostructures in various disciplines can be found in the paper [36] and references cited therein.

This paper is organized as follows. In Section 2, some well-known connectivity indices are given. In Section 3, we describe the molecular construction of $c-WO_3$ nanomultilayer and provide some mathematical formulation of its molecular graph. In Section 4, computations are conducted for $c-WO_3$ nanomultilayer through degree based Zagreb and Randic topological indices with appropriate illustrations. Moreover, In Section 5, we apply some of our results to compare the values of these indices.

2. Preliminaries

In this section, we have enumerated basic definitions of certain topological indices which are needed in framing our work. In mathematical chemistry, most of the topological indices have the form

$$TI = TI(G) = \sum_{u_iu_j \in E(G)} F(d_i, d_j).$$

Definition 2.1 ([13],[14]). *For a simple connected graph G, the first and second Zagreb indices are defined as*

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v), \; M_2(G) = \sum_{uv \in E(G)} (d_u \cdot d_v),$$

where d_v denotes the degree (number of first neighbours) of vertex v in G.

Definition 2.2 ([15]). *Let G be a simple connected graph G, the third Zagreb index is defined as*

$$ZG_3(G) = \sum_{uv \in E(G)} |d_u - d_v|.$$

Definition 2.3 ([16]). *For a simple connected graph G, the first and second hyper Zagreb indices are defined as*

$$HM_1(G) = \sum_{uv \in E(G)} (d_u + d_v)^2, \; HM_2(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)^2.$$

The general case of first and second hyper Zagreb indices are defined as

$$M_1^{\alpha}(G) = \sum_{uv \in E(G)} (d_u + d_v)^{\alpha}, \; M_2^{\alpha}(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)^{\alpha}.$$

Definition 2.4 ([17]). *For a simple connected graph G, the reduced second Zagreb index is defined as*

$$RM_2(G) = \sum_{uv \in E(G)} (d_u - 1) \cdot (d_v - 1).$$

Definition 2.5 ([18]). *For a simple connected graph G, the first, second and third redefined Zagreb indices of G are defined as*

$$\mathrm{Re}ZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v}, \; \mathrm{Re}ZG_2(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v},$$

$$\textit{and } \mathrm{Re}ZG_3(G) = \sum_{uv \in E(G)} (d_u \cdot d_v) \cdot (d_u + d_v).$$

Definition 2.6 ([19]). *Let G be a simple connected graph. The Nano - Zagreb index of G is defined as*

$$\mathcal{N}z(G) = \sum_{uv\in E(G)} \left(d_u^2 - d_v^2\right),$$

with $d_u \gg d_v$.

Definition 2.7 ([20]). *For a simple loopless connected graph G, the sum Nano-Zagreb index of G is defined as*

$$\chi_{\frac{1}{2}}\mathcal{N}z(\mathrm{G}) = \sum_{uv\in E(G)} \left(d_u^2 - d_v^2\right)^{\frac{1}{2}},$$

with $d_u \gg d_v$.

Definition 2.8 ([6]). *For a simple connected graph G, Randić index of G is defined as*

$$R_{-\frac{1}{2}}(\mathrm{G}) = \sum_{uv\in E(G)} (d_u \cdot d_v)^{\frac{-1}{2}}.$$

Definition 2.9 ([21]). *Let G be a simple connected graph. The Reciprocal Randić index is denoted by RR(G) and is defined as*

$$\mathrm{RR}(\mathrm{G}) = \sum_{uv\in E(G)} \sqrt{d_u \cdot d_v}.$$

Definition 2.10 ([22]). *For a simple connected graph G, the Reduced Reciprocal Randić index of* G *is defined as*

$$\mathrm{RRR}(\mathrm{G}) = \sum_{uv\in E(G)} \sqrt{(d_u - 1)\cdot(d_v - 1)}.$$

Definition 2.11 ([23]). *For a simple connected graph G, the zeroth - order Randić index of G is defined as*

$$\mathrm{R}^0_{-\frac{1}{2}}(\mathrm{G}) = \sum_{u\in V(G)} (d_u)^{\frac{-1}{2}}.$$

Definition 2.12 ([25-28]). *If* G *is a simple connected graph, then the zeroth - order general Randić index of* G *is defined as*

$$\mathrm{R}^0_{\alpha}(\mathrm{G}) = \sum_{u\in V(G)} (d_u)^{\alpha}$$

and $\alpha \neq 0, 1$.

Definition 2.13 ([24]). *For a simple connected graph G, the modified Randić index of G is defined as*

$$\mathrm{R}'(\mathrm{G}) = \sum_{uv\in E(G)} \frac{1}{\max\{d_u, d_v\}}.$$

3. Discussions

In this section, first we present the step-by-step formation of $c - WO_3$ nanomultilayer and then discuss the partitions of the vertex set and the edge set of its molecular graph.
Formation of WO_3 nanomultilayers are experimentally studied in [37]. Since topological indices play a predominant role in correlating physiochemical properties of the chemical compounds, we eager to find some degree based Zagreb and Randić indices for $c - WO_3$ nanomultilayer through its molecular graph. The pictorial representation of WO_3 molecular formation is shown in Fig. 1. Unit cell and nanolayer structure of $c - WO_3$ are displayed in Fig. 2 (a) and 2 (b) respectively. The typical WO_3 molecular structure clearly indicates that, each tungsten atom with six oxygen atoms in close proximity, and each oxygen atom and two tungsten atoms are closely adjacent, then each tungsten atom is sub-neighbour with another one. Oxygen atoms are in the surface while tungsten atoms in the center as depicted in Fig. 1 and Fig. 2.

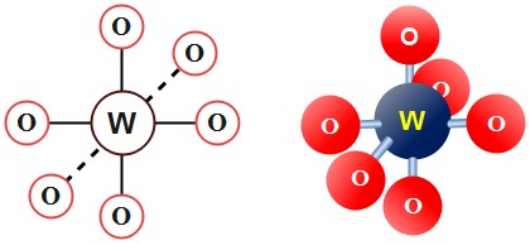

Figure 1. Molecular formation of WO_3 (2-D , 3-D view)

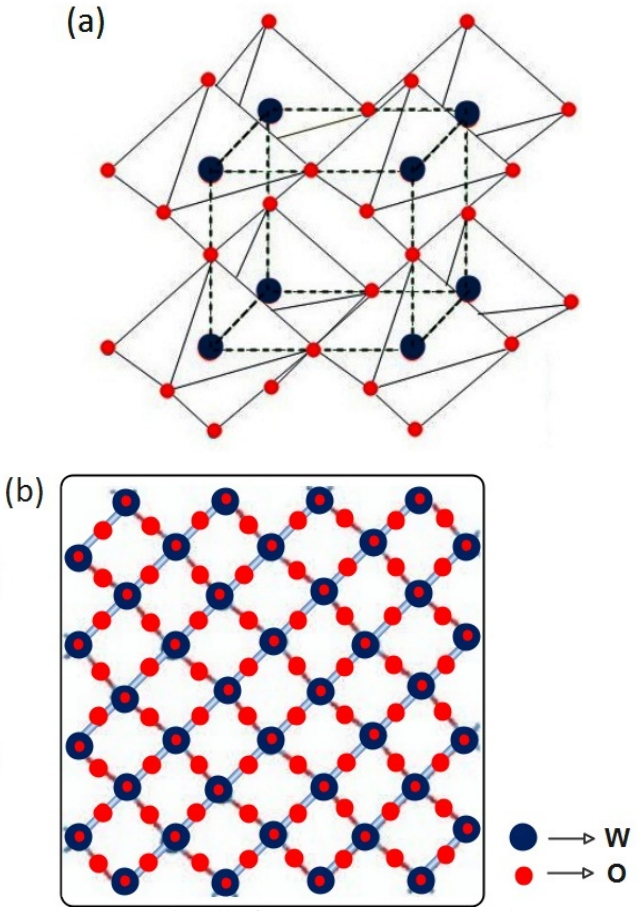

Figure 2. (a) Unit cell of $c - WO_3$ and (b) Nanolayer structure (Top View)

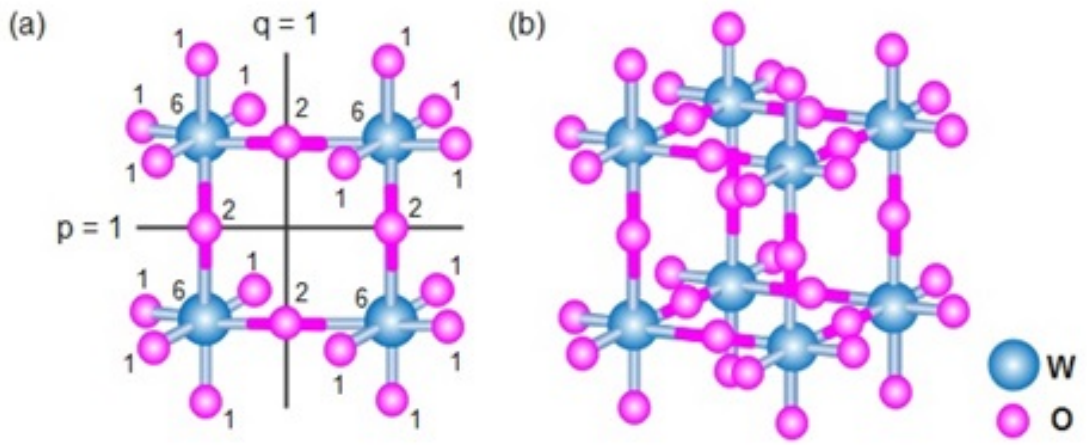

Figure 3. (a) Vertices of $c-WO_3$ [1,1,1] nanomultilayer labelled with degrees 1,2,6 and (b) $c-WO_3$ [1,1,2] nanomultilayer

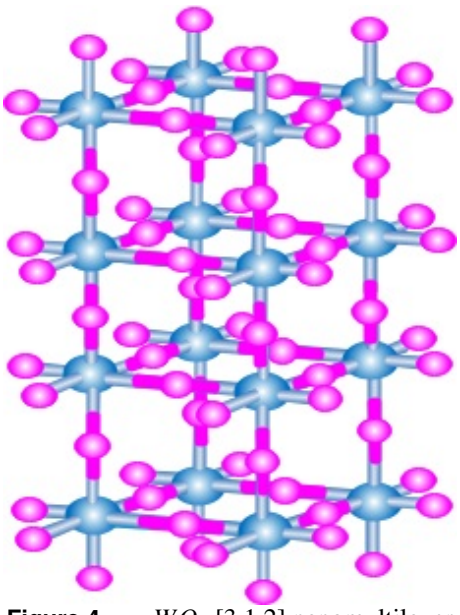

Figure 4. $c-WO_3$ [3,1,2] nanomultilayer

The intermediate space between two horizontal linear arrangements of connected tungsten trioxide molecules is treated as a single row $(p=1)$ in which two tungsten atoms are connected by an oxygen atom. A similar vertical arrangement of this pattern constitutes a single column $(\mathrm{q}=1)$. These two parameters combined together to form a single layer $(\mathrm{r}=1)$. Consider a cubic system of WO_3 nanostructures with p rows, q columns and r layers, and each layer consists of p rows and q columns. Such a typical WO_3 molecular graph W and O atoms displayed as vertices and the bonds connecting them to each other can be represented by edges.There are three types of vertices in $\mathrm{c}-\mathrm{WO}_3$ [p,q,r] nanomultilayer namely of degree 1,2 and 6, and two types of edges with respect to degree of end vertices namely, {1.6} and {2,6} as depicted in Fig. 3 (a). The nanomultilayer of $c-WO_3$ $[1,1,2]$ and $c-WO_3$ $[3,1,2]$ are shown in Fig. 3 (b) and Fig. 4.

Fig. 5 shows the molecular graph of $\mathrm{c}-\mathrm{WO}_3[\mathrm{p},\mathrm{q},\mathrm{r}]$ nanomultilayer (big and small dots indicate W and O atoms respectively). From this, we can observe that the total number of vertices are

$$4pqr+6r+15(pr+qr)+pq+p+q+1$$

and the total number of edges are

$$6r(pq+p+q+1).$$

All surface oxygen atoms connected with tungsten atoms are denoted by the edge type $E_{(1,6)}$ and the intermediated oxygen atoms binded with tungsten atoms are shown by the edge type $E_{(2,6)}$.

The edge set of $\mathrm{c}-\mathrm{WO}_3[\mathrm{p},\mathrm{q},\mathrm{r}]$ nanomultilayer with $p,q,r\geq 1$ has following two partitions,

$$E_{(1,6)}=\{e=uv\in E\,(c-WO_3[p,q,r])\mid d_u=1,d_v=6\}$$

and

$$E_{(2,6)}=\{e=uv\in E\,(c-WO_3[p,q,r])\mid d_u=2,d_v=6\}$$

The vertex set of $\mathrm{c}-\mathrm{WO}_3[\mathrm{p},\mathrm{q},\mathrm{r}]$ nanomultilayer with $p,q,r\geq 1$ has following three partitions,

$$V_1=\{v\in V\,(c-WO_3[p,q,r])\mid d_v=1\},$$

$$V_2=\{v\in V\,(c-WO_3[p,q,r])\mid d_v=2\}$$

and

$$V_6=\{v\in V\,(c-WO_3[p,q,r])\mid d_v=6\}$$

Edge partition and Vertex partition of $\mathrm{c}-\mathrm{WO}_3$ [p,q,r] nanomultilayer based on the degree of end vertices of each edge in r layers are given in Table 1 and Table 2.

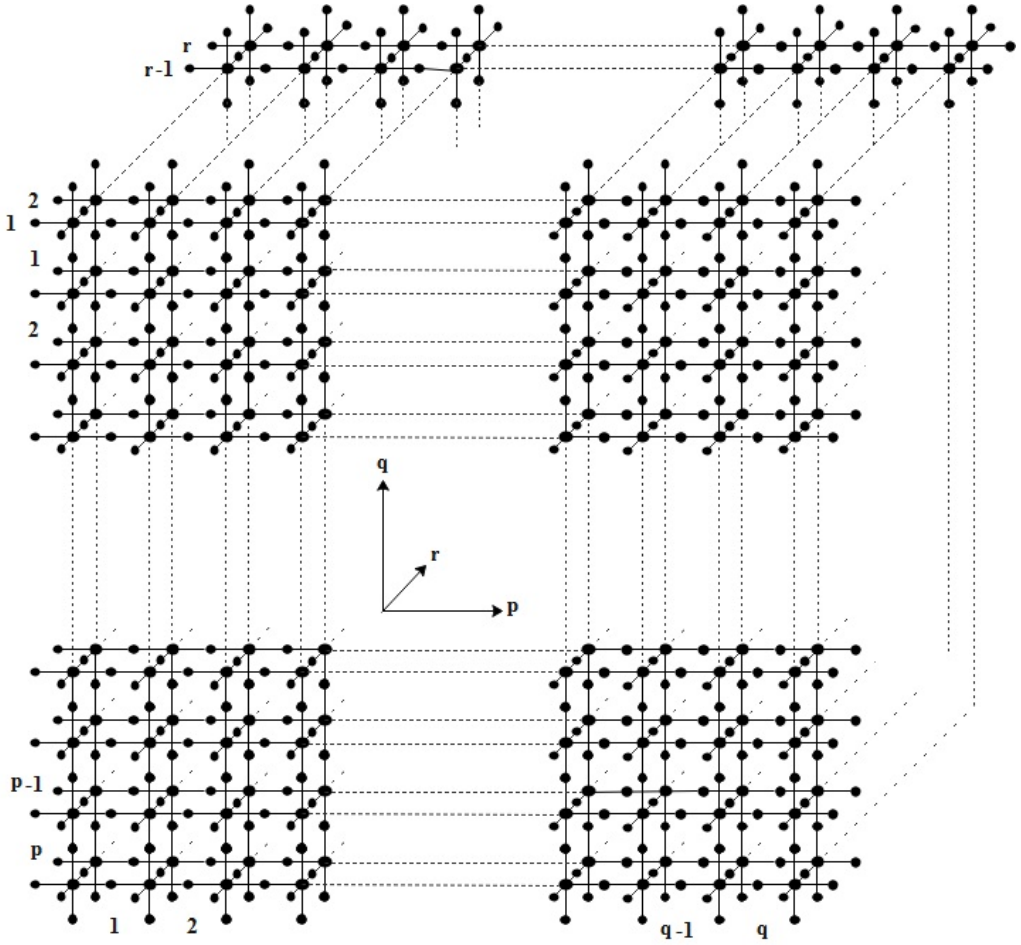

Figure 5. Molecular graph of $c-WO_3$ $[p,q,r]$ nanomultilayer

Table 1. Edge partition of $c-WO_3$ [p,q,r] nanomultilayer based on the degree of end vertices of each edge in r layers

Type of edges	$E_{(1,6)}$	$E_{(2,6)}$
$(d_u,d_v), uv \in E(G)$	(1,6)	(2,6)
Edge cardinality $\mid E_{(d_u,d_v)} \mid$	$2(pq+qr+rp+p+q+2r+1)$	$6pqr+4(pr+qr)+2r$ $-2(pq+p+q+1)$

4. Main Results

In this section, we present accurate expression of several degree based Zagreb and Randić indices of $c-WO_3$[p,q,r] nanomultilayer by edge partition technique.

Theorem 4.1. *For all p, q, r* ≥ 1*, The first Zagreb index of* $c-WO_3$ *[p,q,r] nanomultilayer is given by*

$$\begin{aligned} M_1(c-WO_3[p,q,r]) =& 48pqr+46(pr+qr) \\ &+2(22r-pq) \\ &-2(p+q+1). \end{aligned}$$

Proof. Using Table 1 and the mathematical expression of first Zagreb index $M_1(G)=\sum_{uv\in E(G)}(d_u+d_v)$, we get

$$\begin{aligned} &M_1(c-WO_3[p,q,r]) \\ &=|E_{(1,6)}|(1+6)+|E_{(2,6)}|(2+6) \\ &=2(pq+qr+rp+p+q+2r+1)(7) \\ &\quad +8(6pqr+4(pr+qr)+2r-2(pq+p+q+1)) \\ &=48pqr+46(pr+qr)+2(22r-pq)-2(p+q+1). \end{aligned}$$

□

Example 4.2. *Consider a 3D structure of* $c-WO_3[5,4,3]$ *nanomultilayer consisting of 423 atoms and 540 chemical bonds, we obtain,*

$$M_1(c-WO_3[5,4,3]) = 4194.$$

Table 2. Vertex partition of $c-WO_3\ [p,q,r]$ nanomultilayer based on the degree of end vertices of each edge in r layers

Vertex partition V_{d_u}	V_1	V_2	V_6
$d_u, u \in V(G)$	1	2	6
Vertex cardinality $\lvert V_{d_u}\rvert$	$2(pq+qr+rp+p+q+2r+1)$	$3pqr+2(pr+qr)$ $-(pq+p+q+r+1)$	$(pq+p+q+1)r$

Theorem 4.3. *For all p, q, r ≥ 1, the second Zagreb index of $c-WO_3\ [p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}\mathrm{M_2\,(c-WO_3[p,q,r])} =& 72\mathrm{pqr}+60(\mathrm{pr}+qr)\\ &+12(4r-pq)-12(p+q+1).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of second Zagreb index $M_2(G)=\sum_{uv\in E(G)}(d_u\cdot d_v)$, we get

$$\begin{aligned}&M_2\,(c-WO_3[p,q,r])\\ &=\left|E_{(1,6)}\right|(1\times 6)+\left|E_{(2,6)}\right|(2\times 6)\\ &=2(pq+qr+rp+p+q+2r+1)(6)\\ &\quad+12(6pqr+4(pr+qr)+2r-2(pq+p+q+1))\\ &=72pqr+60(pr+qr)+12(4r-pq)-12(p+q+1).\end{aligned}$$

□

Example 4.4. *Consider a 3D structure of $c-WO_3[17,45,76]$ nanomultilayer consisting of 257404 atoms and 377568 chemical bonds, we obtain,*

$$\mathrm{M_2\,(c-WO_3[17,45,76])} = 4462512.$$

Theorem 4.5. *For all p, q, r ≥ 1, the third Zagreb index of $c-WO_3\ [p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}\mathrm{M_2\,(c-WO_3[p,q,r])} =& 24\mathrm{pqr}+26(\mathrm{pr}+qr)\\ &+2(14r+pq)+2(p+q+1).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of third Zagreb index $\mathrm{ZG_3(G)}=\sum_{uv\in E(G)}|d_u-d_v|$, we get

$$\begin{aligned}&ZG_3\,(c-WO_3[p,q,r])\\ &=|E_{(1,6)}||1-6|+\left|E_{(2,6)}\right||2-6|\\ &=2(pq+qr+rp+p+q+2r+1)(5)\\ &\quad+(6pqr+4(pr+qr)+2r-2(pq+p+q+1))(4)\\ &=24pqr+26(pr+qr)+2(14r+pq)+2(p+q+1).\end{aligned}$$

□

Example 4.6. *Consider a 3 D structure of $c-WO_3[54,78,48]$ nanomultilayer consisting of 845017 atoms and 1021554 chemical bonds, we obtain,*

$$\mathrm{ZG_3\,(c-WO_3[54,78,48])} = 5026994.$$

Theorem 4.7. *For all $p,q,r\geq 1$ the first hyper Zagreb index of $c-WO_3\ [p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}\mathrm{HM_1\,(c-WO_3[p,q,r])} &= 384\mathrm{pqr}\\ &+354(pr+qr)+3(108r-10pq)-30(p+q+1).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of first hyper Zagreb index $HM_1(G)=\sum_{uv\in E(G)}(d_u+d_v)^2$ we get

$$\begin{aligned}&\mathrm{HM_1\,(c-WO_3[p,q,r])}\\ &=\left|E_{(1,6)}\right|(1+6)^2+\left|E_{(2,6)}\right|(2+6)^2\\ &=98(pq+qr+rp+p+q+2r+1)+64(6pqr\\ &\quad+4(pr+qr)+2r-2(pq+p+q+1))\\ &=384pqr+354(pr+qr)+3(108r-10pq)\\ &\quad-30(p+q+1).\end{aligned}$$

□

Example 4.8. *Consider a 3D structure of $c-WO_3\ [57,88,65]$ nanomultilayer consisting of 1356837 atoms and 2029434 chemical bonds, we obtain,*

$$\mathrm{HM_1\,(c-WO_3[57,88,65])} = 1.3\times 10^8.$$

Theorem 4.9. *For all $p,q,\ r\geq 1$, the second hyper Zagreb index of $c-WO_3\ [\mathrm{p,q,r}]$ nanomultilayer is given by*

$$\begin{aligned}\mathrm{HM_2\,(c-WO_3[p,q,r])} =& 864\mathrm{pqr}+648(pr+qr)\\ &+72(6r-3pq)-216(p+q+1).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of second hyper Zagreb index $HM_2(G)=\sum_{uv\in E(G)}(d_u\cdot d_v)^2$, we get

$$\begin{aligned}&\mathrm{HM_2\,(c-WO_3[p,q,r])}\\ &=\left|E_{(1,6)}\right|(1\times 6)^2+\left|E_{(2,6)}\right|(2\times 6)^2\\ &=72(pq+qr+rp+p+q+2r+1)+144(6pqr\\ &\quad+4(pr+qr)+2r-2(pq+p+q+1))\\ &=864pqr+648(pr+qr)\\ &\quad+72(6r-3pq)-216(p+q+1).\end{aligned}$$

□

Example 4.10. *Consider a 3D structure of $c-WO_3\ [24,46,76]$ nanomultilayer consisting of 363847 atoms and 535800 chemical bonds, we obtain,*

$$HM_2\,(\mathrm{c-WO_3[24,46,76]}) = 7.6\times 10^7.$$

Theorem 4.11. *For all $p,q,r \geq 1$, the general case of first hyper Zagreb index of $c-WO_3$ $[p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}&{M_1}^{\alpha}(\mathrm{c-WO_3[p,q,r]})\\&=2(pq+qr+rp+p+q+2r+1)(7)^{\alpha}\\&\quad+(6pqr+4(pr+qr)+2r-2(pq+p+q+1))(8)^{\alpha}.\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of general case of first hyper Zagreb index

$$M_1^{\alpha}(G)=\sum_{uv\in E(G)}(d_u+d_v)^{\alpha},$$

we get

$$\begin{aligned}&M_1^{\alpha}(\mathrm{c-WO_3[p,q,r]})\\&=\left|E_{(1,6)}\right|(1+6)^{\alpha}+\left|E_{(2,6)}\right|(2+6)^{\alpha}\\&=2(pq+qr+rp+p+q+2r+1)(7)^{\alpha}\\&\quad+(6pqr+4(pr+qr)+2r-2(pq+p+q+1))(8)^{\alpha}.\end{aligned}$$

□

Theorem 4.12. *For all* $\mathrm{p,q,r} \geq 1$, *the general case of second hyper Zagreb index of* $\mathrm{c-WO_3[p,q,r]}$ *nanomultilayer is given by*

$$\begin{aligned}&{M_2}^{\alpha}(\mathrm{c-WO_3[p,q,r]})\\&=2(pq+qr+rp+p+q+2r+1)(6)^{\alpha}\\&\quad+(6pqr+4(pr+qr)\\&\quad+2r-2(pq+p+q+1))(12)^{\alpha}.\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of general case of second hyper Zagreb index

$$M_2^{\alpha}(G)=\sum_{uv\in E(G)}(d_u\cdot d_v)^{\alpha},$$

we get

$$\begin{aligned}&M_2^{\alpha}(\mathrm{c-WO_3[p,q,r]})\\&=\left|E_{(1,6)}\right|(1\times 6)^{\alpha}+\left|E_{(2,6)}\right|(2\times 6)^{\alpha}\\&=2(pq+qr+rp+p+q+2r+1)(6)^{\alpha}\\&\quad+(6pqr+4(pr+qr)\\&\quad+2r-2(pq+p+q+1))(12)^{\alpha}.\end{aligned}$$

□

Theorem 4.13. *For all p, $q,r \geq 1$, the Reduced second Zagreb index of $c-WO_3[p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}&\mathrm{RM_2(c-WO_3[p,q,r])}\\&\quad=30pqr+20(pr+qr)+10(r-pq-p-q-1).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of Reduced second Zagreb index $RM_2(G)=\sum_{uv\in E(G)}(d_u-1)\cdot(d_v-1)$, we get

$$\begin{aligned}&\mathrm{RM_2(c-WO_3[p,q,r])}\\&=\left|E_{(1,6)}\right|(1-1)\cdot(6-1)+\left|E_{(2,6)}\right|(2-1)\cdot(6-1)\\&=2(pq+qr+rp+p+q+2r+1)(0)\\&\quad+5(6pqr+4(pr+qr)+2r-2(pq+p+q+1))\\&=30pqr+20(pr+qr)+10(r-pq-p-q-1).\end{aligned}$$

□

Example 4.14. *Consider a 3D structure of$c-WO_3[10,7,9]$ nanomultilayer consisting of* 3427 *atoms and 4752 chemical bonds, we obtain,* $\mathrm{M_3(c-WO_3[10,7,9])}=21170$.

Theorem 4.15. *For all $p,q,\ r \geq 1$, the first Redefined Zagreb index of c - WO_3 $[p,q,\ r]$ nanomultilayer is given by*

$$\begin{aligned}&\mathrm{ReZG_1(c-WO_3[p,q,r])}\\&\quad=4pqr+5(pr+qr)+(6r+pq)+(p+q+1).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of first Redefined Zagreb index

$$\mathrm{ReZG_1}(G)=\sum_{uv\in E(G)}\frac{d_u+d_v}{d_u\cdot d_v},$$

we get

$$\begin{aligned}&\mathrm{ReZG_1(c-WO_3[p,q,r])}\\&=\left|E_{(1,6)}\right|\left(\frac{1+6}{1\times 6}\right)+\left|E_{(2,6)}\right|\left(\frac{2+6}{2\times 6}\right)\\&=\frac{7}{3}(pq+qr+rp+p+q+2r+1)+\frac{2}{3}(6pqr\\&\quad+4(pr+qr)+2r-2(pq+p+q+1))\\&=4pqr+5(pr+qr)+(6r+pq)+(p+q+1).\end{aligned}$$

□

Example 4.16. *Consider a 3D structure of $c-WO_3[5,8,5]$ nanomultilayer consisting of 1209 atoms and 1620 chemical bonds, we obtain,* $\mathrm{ReZG_1}\,(c-WO_3[5,8,5])=1209$.

Theorem 4.17. *For all $p,q,r \geq 1$, the second Redefined Zagreb index of $c-WO_3[p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}&\mathrm{ReZG_2(c-WO_3[p,q,r])}\\&\quad=9pqr+7.7143(pr+qr)+(6.4285r-1.2857pq)\\&\quad-1.2857(p+q+1).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of second Redefined Zagreb index $\mathrm{ReZG_2}(G)=\sum_{uv\in E(G)}\frac{d_u\cdot d_v}{d_u+d_v}$,

we get

$$\begin{aligned}&\mathrm{Re}ZG_2\,(\mathrm{c}-\mathrm{WO_3[p,q,r]})\\&=\left|E_{(1,6)}\right|\left(\frac{1\cdot 6}{1+6}\right)+\left|E_{(2,6)}\right|\left(\frac{2\cdot 6}{2+6}\right)\\&=\frac{12}{7}(pq+qr+rp+p+q+2r+1)\\&\quad+\frac{12}{8}(6pqr+4(pr+qr)\\&\quad+2r-2(pq+p+q+1))\\&=9pqr+7.7143(pr+qr)+(6.4285r-1.2857pq)\\&\quad-1.2857(p+q+1).\end{aligned}$$

□

Example 4.18. *Consider a 3D structure of $c-WO_3$ $[10,8,5]$ nanomultilayer consisting of 2179 atoms and 2970 chemical bonds, we obtain,* $\mathrm{Re}ZG_2\,(c-WO_3[10,8,5])=4199.143$.

Theorem 4.19. *For all $p,\ q,r\geq 1$, the third Redefined Zagreb index of $c-WO_3[p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}&\mathrm{Re}ZG_3\,(\mathrm{c}-\mathrm{WO_3[p,q,r]})\\&=576pqr+468(pr+qr)+24(15r-4.5pq)\\&\quad-108(p+q+1).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of third Redefined Zagreb index

$$\mathrm{Re}ZG_3(\mathrm{G})=\sum_{uv\in E(G)}(d_u\cdot d_v)\cdot(d_u+d_v),$$

we get

$$\begin{aligned}&Re\mathrm{ZG_3}\,(\mathrm{c}-\mathrm{WO_3[p,q,r]})\\&=\left|E_{(1,6)}\right|(6)(1)\cdot(6+1)+\left|E_{(2,6)}\right|(6)(2)\cdot(6+2)\\&=84(pq+qr+rp+p+q+2r+1)\\&\quad+96(6pqr+4(pr+qr)+2r-2(pq+p+q+1))\\&=576pqr+468(pr+qr)+24(15r-4.5pq)\\&\quad-108(p+q+1).\end{aligned}$$

□

Example 4.20. *Consider a 3D structure of $c-WO_3[10,6,5]$ nanomultilayer consisting of 1707 atoms and 2310 chemical bonds, we obtain,*

$$\mathrm{Re}ZG_3\,(\mathrm{c}-\mathrm{WO_3[10,6,5]})=203724.$$

Theorem 4.21. *For all $p,q,\ r\geq 1$, the Nano - Zagreb index of $c-WO_3$ $[p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}&\mathcal{N}z(c-\mathrm{WO_3[p,q,r]})\\&=192\mathrm{pqr}+198(\mathrm{pr}+qr)+6(34r+pq)+6(p+q+1).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of the Nano - Zagreb index

$$\mathcal{N}z(G)=\sum_{uv\in E(G)}\left(d_u^2-d_v^2\right),\ \text{with } d_u\gg d_v,$$

we get

$$\begin{aligned}&\mathcal{N}z(c-\mathrm{W03[p,q,r]})\\&=\left|E_{(1,6)}\right|\left(6^2-1^2\right)+\left|E_{(2,6)}\right|\left(6^2-2^2\right)\\&=70(pq+qr+rp+p+q+2r+1)+32(6pqr\\&\quad+4(pr+qr)+2r-2(pq+p+q+1))\\&=192pqr+198(pr+qr)+6(34r+pq)\\&\quad+6(p+q+1).\end{aligned}$$

□

Example 4.22. *Consider a 3D structure of $c-WO_3[10,8,15]$ nanomultilayer consisting of 6339 atoms and 8910 chemical bonds, we obtain,* $\mathcal{N}z\,(c-WO_3\,[10,8,15])=287514$.

Theorem 4.23. *For all $p,q,\ r\geq 1$, the Sum Nano - Zagreb index of $c-WO_3\,[p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}&\chi_{\frac{1}{2}}\mathcal{N}z\,(\mathrm{c}-\mathrm{WO_3[p,q,r]})\\&=2(pq+qr+rp+p+q+2r+1)(35)^{\frac{1}{2}}\\&\quad+(6pqr+4(pr+qr)+2r\\&\quad-2(pq+p+q+1))(32)^{\frac{1}{2}}.\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of Sum Nano-Zagreb index $\chi_{\frac{1}{2}}\mathcal{N}z(\mathrm{G})=\sum_{uv\in E(G)}\left(d_u^2-d_v^2\right)^{\frac{1}{2}}$, with $d_u\gg d_v$, we get

$$\begin{aligned}&\chi_{\frac{1}{2}}\mathcal{N}z\,(\mathrm{c}-\mathrm{WO_3[p,q,r]})\\&=\left|E_{(1,6)}\right|\left(6^2-1^2\right)^{\frac{1}{2}}+\left|E_{(2,6)}\right|\left(6^2-2^2\right)^{\frac{1}{2}}\\&=2(pq+qr+rp+p+q+2r+1)(35)^{\frac{1}{2}}\\&\quad+(6pqr+4(pr+qr)+2r\\&\quad-2(pq+p+q+1))(32)^{\frac{1}{2}}.\end{aligned}$$

□

Example 4.24. *Consider a 3D structure of $c-WO_3$ $[15,18,5]$ nanomultilayer consisting of 6559 atoms and 9120 chemical bonds, we obtain,*

$$\chi_{\frac{1}{2}}\mathcal{N}z\,(\mathrm{c}-\mathrm{WO_3[15,18,5]})=51838.8488.$$

Theorem 4.25. *For all $p,q,r\geq 1$, the Randić index of $c-WO_3[p,q,r]$ nanomultilayer is given by*

$$\begin{aligned}&R_{\frac{-1}{2}}\,(WO_3[\mathrm{p,q,r}])=2(pq+qr+rp+p+q+2r+1)/\sqrt{6}\\&\quad+((6pqr+4(pr+qr)+2r-2(pq+p+q+1)))/(2\sqrt{3}).\end{aligned}$$

Proof. Using Table 1 and the mathematical expression of Randić index $R_{-\frac{1}{2}}(\mathrm{G}) = \sum_{uv\in E(G)} (d_u \cdot d_v)^{\frac{-1}{2}}$, we get

$$\begin{aligned} R_{\frac{-1}{2}}(WO_3[\mathrm{p,q,r}]) &= \left|E_{(1,6)}\right| (1\times 6)^{\frac{-1}{2}} + \left|E_{(2,6)}\right| (2\times 6)^{\frac{-1}{2}} \\ &= (2(pq+qr+rp+p+q+2r+1))/\sqrt{6} \\ &\quad +((6pqr+4(pr+qr)+2r-2(pq+p+q+1)))/(2\sqrt{3}). \end{aligned}$$

□

Example 4.26. *Consider a 3D structure of* $c-WO_3$ $[10,7,4]$ *nanomultilayer consisting of 1572 atoms and 2112 chemical bonds, we obtain,* $R_{\frac{-1}{2}}(\mathrm{c-WO_3}[10,7,4]) = 648.901879$.

Theorem 4.27. *For all* $p,q,r \geq 1$*, the Reciprocal Randić index of* $c-WO_3$ $[p,q,r]$ *nanomultilayer is given by*

$$\begin{aligned} &\mathrm{RR}(\mathrm{c-WO_3[p,q,r]}) \\ &=2\sqrt{6}(pq+qr+rp+p+q+2r+1) \\ &\quad +2\sqrt{3}(6pqr+4(pr+qr)+2r-2(pq+p+q+1)). \end{aligned}$$

Proof. Using Table 1 and the mathematical expression of the Reciprocal Randić index

$$\mathrm{RR(G)} = \sum_{uv\in E(G)} \sqrt{d_u \cdot d_v},$$

we get

$$\begin{aligned} \mathrm{RR}(\mathrm{c-WO_3[p,q,r]}) &= \left|E_{(1,6)}\right| \sqrt{1\cdot 6} + \left|E_{(2,6)}\right| \sqrt{2\cdot 6} \\ &= 2(pq+qr+rp+p+q+2r+1)\sqrt{6} \\ &\quad +\sqrt{12}(6pqr+4(pr+qr)+2r-2(pq+p+q+1)) \\ &= 2\sqrt{6}(pq+qr+rp+p+q+2r+1) \\ &\quad +2\sqrt{3}(6pqr+4(pr+qr)+2r-2(pq+p+q+1)). \end{aligned}$$

□

Example 4.28. *Consider a 3D structure ofc* $-WO_3[10,5,5]$ *nanomultilayer consisting of 1471 atoms and 1980 chemical bonds, we obtain,* $\mathrm{RR}(\mathrm{c-WO_3}[10,5,5]) = 6552.50841$.

Theorem 4.29. *For all p, q,* $r \geq 1$*, the Reduced Reciprocal Randić index of* $\mathrm{c-WO_3[p,q,r]}$ *nanomultilayer is given by*

$$\begin{aligned} \mathrm{RRR}(\mathrm{c-WO_3[p,q,r]}) =& \sqrt{5}(6pqr+4(pr+qr)+2r \\ &-2(pq+p+q+1)). \end{aligned}$$

Proof. Using Table 1 and the mathematical expression of the Reduced Reciprocal Randić index

$$\mathrm{RRR(G)} = \sum_{uv\in E(G)} \sqrt{(d_u-1)\cdot(d_v-1)},$$

we get

$$\begin{aligned} &RRR(\mathrm{c-WO_3[p,q,r]}) \\ &= \left|E_{(1,6)}\right| \sqrt{(1-1)(6-1)} + \left|E_{(2,6)}\right| \sqrt{(2-1)(6-1)} \\ &=2(pq+qr+rp+p+q+2r+1)\sqrt{(0)\cdot(5)} \\ &\quad +\sqrt{(1)\cdot(5)}(6pqr+4(pr+qr) \\ &\quad +2r-2(pq+p+q+1)) \\ &=\sqrt{5}(6pqr+4(pr+qr)+2r-2(pq+p+q+1)). \end{aligned}$$

□

Example 4.30. *Consider a 3D structure of* $c-WO_3$ $[10,18,5]$ *nanomultilayer consisting of 4539 atoms and 6270 chemical bonds, we obtain,* $\mathrm{RRR}(\mathrm{c-WO_3}[10,18,5]) = 12414.6494$.

Theorem 4.31. *For all* $p,q,r \geq 1$*, the zeroth - order Randić index of* $\mathrm{c-}WO_3$ $[\mathrm{p,q,r}]$ *nanomultilayer is given by*

$$\begin{aligned} R^0_{\frac{-1}{2}}(c-WO3[p,q,r]) &= 2(pq+qr+rp+p+q+2r+1) \\ &\quad + \frac{3pqr+2(pr+qr)-(pq+p+q+r+1)}{\sqrt{2}} \\ &\quad + \frac{(pq+p+q+1)r}{\sqrt{6}}. \end{aligned}$$

Proof. Using Table 2 and the mathematical expression of the zeroth-order Randić index, $\mathrm{R}^0_{-\frac{1}{2}}(\mathrm{G}) = \sum_{u\in V(G)} (d_u)^{\frac{-1}{2}}$, we get

$$\begin{aligned} R^0_{-\frac{1}{2}}(c-WO_3[p,q,r]) &= |V_1|(1)^{\frac{-1}{2}} + |V_2|(2)^{\frac{-1}{2}} + |V_6|(6)^{\frac{-1}{2}} \\ &=2(pq+qr+rp+p+q+2r+1) \\ &\quad + \frac{3pqr+2(pr+qr)-(pq+p+q+r+1)}{\sqrt{2}} \\ &\quad + \frac{(pq+p+q+1)r}{\sqrt{6}}. \end{aligned}$$

□

Example 4.32. *Consider a 3D structure of* $c-WO_3[3,8,4]$ *nanomultilayer consisting of 664 atoms and 864 chemical bonds, we obtain,* $R^0_{\frac{-1}{2}}(\mathrm{c-WO_3}[3,8,4]) = 478.032487$.

Theorem 4.33. *For all* $p,q,r \geq 1$*, the zeroth - order general Randić index of* $c-WO_3[p,q,r]$ *nanomultilayer is given by*

$$\begin{aligned} &R^0_\alpha(c-WO3[p,q,r]) \\ &=2(pq+qr+rp+p+q+2r+1)(1)^\alpha \\ &\quad +(3pqr+2(pr+qr)-(pq+p+q+r+1))(2)^\alpha \\ &\quad +((pq+p+q+1)r)(6)^\alpha, \end{aligned}$$

where α *is a real number other than* 0 *and* 1.

Proof. Using Table 2 and the mathematical expression of the zeroth-order general Randić index $R^0_\alpha(G) = \sum_{u\in V(G)} (d_u)^\alpha$ and $\alpha \neq 0,1$, we get

$$\begin{aligned} &R^0_\alpha(c-WO3[p,q,r]) \\ &=|V_1|(1)^\alpha + |V_2|(2)^\alpha + |V_6|(6)^\alpha \\ &=2(pq+qr+rp+p+q+2r+1)(1)^\alpha \\ &\quad +(3pqr+2(pr+qr)-(pq+p+q+r+1))(2)^\alpha \\ &\quad +((pq+p+q+1)r)(6)^\alpha. \end{aligned}$$

□

Theorem 4.34. *For all $p,q,r \geq 1$, the modified Randić index of $c-WO_3$ $[p,q,r]$ nanomultilayer is given by*

$$\begin{aligned} &R'(c-WO_3[p,q,r]) \\ &= \frac{2(pq+qr+rp+p+q+2r+1)}{6} \\ &\quad + \frac{6pqr+4(pr+qr)+2r-2(pq+p+q+1)}{6}. \end{aligned}$$

Proof. Using Table 1 and the mathematical expression of the modified Randić index $R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_u,d_v\}}$, we get

$$\begin{aligned} &R'(c-WO_3[p,q,r]) \\ &= |E_{(1,6)}| \frac{1}{\max\{1,6\}} + |E_{(2,6)}| \frac{1}{\max\{2,6\}} \\ &= \frac{2(pq+qr+rp+p+q+2r+1)}{6} \\ &\quad + \frac{6pqr+4(pr+qr)+2r-2(pq+p+q+1)}{6}. \end{aligned}$$

□

Example 4.35. *Consider a 3D structure ofc $-WO_3[7,8,6]$ nanomultilayer consisting of 1902 atoms and 2592 chemical bonds, we obtain, R' (c $-$ WO$_3$[7,8,6]) $= 432$.*

5. Comparative Analysis

In this section, we present graphs (Figures 6–8) with key features that exhibit the trends of dependency among the values of indices and the number of vertices expressed in terms of the parameters $[p,q,r]$.
All indices disclose an upward trend with the increase in the dimension of c $-$ WO$_3$[p,q,r] nanomultilayer. Plotting the values of indices in graphs, the following observations have been made:

(i) $ZG_3(G) < M_1(G) < M_2(G) < HM_l(G) < HM_2(G)$

(ii) $\mathrm{Re}ZG_1(G) < \mathrm{Re}ZG_2(G) < RM_2(G) < \mathrm{Re}ZG_3(G)$

(iii) $\mathrm{R}'(\mathrm{G}) < \mathrm{R}_{-1/2}(G) < \mathrm{R}^0_{-1/2}(G) < RRR(G) < RR(G)$

(iv) $\chi_{1/2}\mathcal{N}z(G) < \mathcal{N}z(G)$

(v) $RR(G) < \mathcal{N}z(G) < ReZG_3(G) < HM_2(G)$.

It is evident that, Second hyper Zagreb index (HM$_2$(G)) increases sharply as compared to other indices. It is now an established fact that total π - electron energy of chemical compounds is closely related with Zagreb indices [14,38], hence it can be concluded that this energy will rise with the rise in dimension.

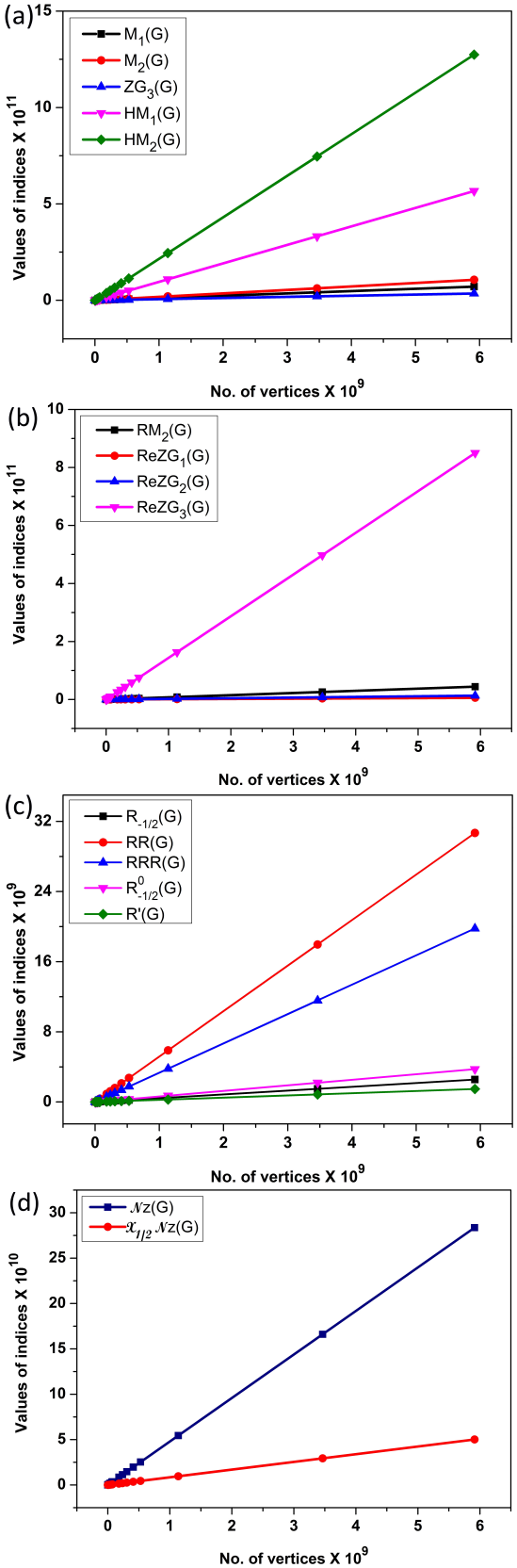

Figure 6. A comparison of various topological indices (a) $M_l(G), M_2(G), ZG_3(G), HM_l(G)$ and $HM_2(G)$ (b) $RM_2(G), \mathrm{Re}ZG_l(G), \mathrm{Re}ZG_2(G)$ and $\mathrm{Re}ZG_3(G)$ (c) $R_{-1/2}(G), RR(G), RRR(G), R^0_{-1/2}(G)$ and $\mathrm{R}'(\mathrm{G})$ and (d) $\mathcal{N}z(G)$ and $\mathcal{X}_{1/2}\mathcal{N}z(G)$ of $c-WO_3[p,q,r]$ nanomultilayer

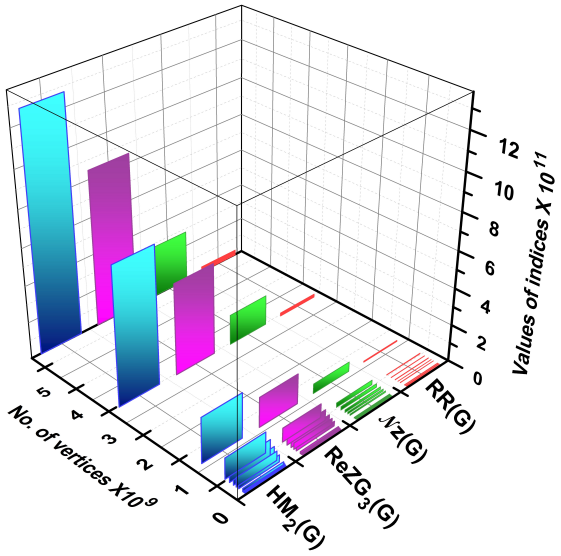

Figure 7. A $3-D$ plot showing the comparison of $HM_2(G)$, $\mathrm{Re}ZG_3(G)$, $\mathscr{N}z(G)$ and $RR(G)$ of $\mathrm{c-WO_3[p,q,r]}$ nanomultilayer

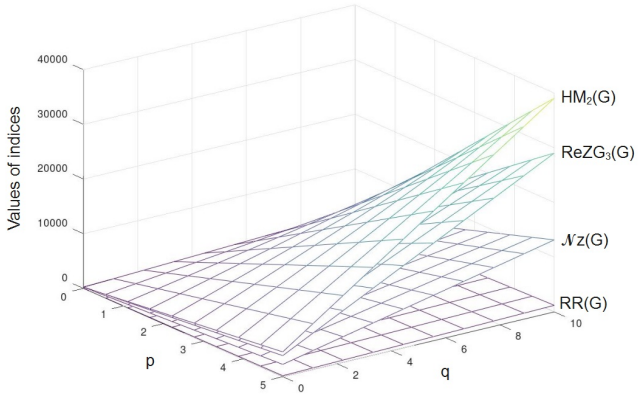

Figure 8. A $3-D$ surface plot of $c-WO_3$ $[p,q,r]$ monolayer with $p \in [1,5]$ and $q \in [1,10]$ using Octave software.

6. Conclusion

In this article, many important degree based Zagreb and Randić indices for $\mathrm{c-WO_3[p,q,r]}$ nanomultilayer were established and computed analytically for all possible values of the parameters p, q and r. As we discussed the key outcomes of the reported indices, it is clear that the expectation of this study has been amply manifested. We also demonstrated the comparison among the indices discussed in this article. This interdisciplinary approach will shed light on the significance of mathematical formulation in chemical physics. This could be a better opportunity to reveal new insights in $3-D\mathrm{WO_3}$ nanostructures through graph theoretic approach. The other useful topological indices like ABC, GA, SK, SCI and AZI will be discussed in our subsequent work.

Declarations

Conflict of interests

The authors declare that there is no conflict of interests.

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