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Research article

Comparative study of vertex-edge based indices for semi-capped carbon nanotubes

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Abstract: Manufacturing relatively inexpensive items in every area of engineering and science is the major focus of exploration resultant the world's contemporary economic setback. Making small-sized items that are inexpensive and lightweight while providing high quality is critical in today's and tomorrow's worlds. Nanotechnology has a significant role to play in this situation. Nano-objects or, in general, nanomaterials are especially preferred; nanotubes, especially those comprised of carbon, are one of the most popular types of nanostructures, and they are applied in a variety of chemical, biological and technical applications. This notion prompted us to investigate their many physical and chemical characteristics. We utilized topological descriptors to evaluate diverse nanotube structures such as armchair carbon and semi-capped nanotubes by using vertex-edge based indices to characterize distinct chemical structures via numerical quantitative analysis. Furthermore, we examined uncapped and semi-capped armchair carbon nanotubes and achieved adequate comparative findings.

Keywords: *ev*-degree; topological indices; carbon nanotubes; carbon capped nanotubes; carbon semi-capped nanotubes

1. Introduction

Carbon nanotubes have been widely used in research since their initial development by the authors of [1]. Carbon nanotubes are remarkable compounds as compared to others. Their thermal conductivity is higher than that of other materials, and their electrical conductivity is comparable to copper.

According to the manufacturer, they are more robust, can tackle larger currents and have a much better tensile strength than steel [2].

Carbon nanotubes that are capped or semi-capped are one of the nanotube types. For distinct armchair carbon nanotube symmetries, semi-capped implies one-end open nanotubes, whereas capped refers to both-end closed nanotubes [3]. While carbon nanotubes are well-known for their applications, semi-capped and capped nanotubes are equally valuable in a variety of scientific fields. The overall uses of semi-capped, capped and carbon nanotubes are presented in the following literature: the detection of subsurface defects [4], a material in photovoltaics and saturable absorbers [5], thin films [6] fuel cells [7], a material for CVD growth with a palm oil precursor [8], applications in regenerative medicine and pharmaceuticals [9], as a memory device [10], a material in tissue and biomedical engineering [11, 12], a material for self-cleaning solar cell coating and anti-reflection [13], a material to immobilize and improve the function of certain biomolecules [14], a material in biochemical sensors for the analysis of pyrophosphate, cholesterol, lactate, glucose, alcohols and other analytes [15], carbon nanotubes are used in the applications of DNA and proteins and found in [16]. Additionally, for nanostructure details, particularly carbon nanotubes, we refer the reader to [17–20]; also, apart from the applications listed above, we recommend [21–25].

Limited to the scope of the paper, we recommend [24,25] for more information on chiral and zigzag nanotubes. The nanotubes divided into single- and multi-walled nanotubes resulting from the drifting of single- and multi-walled sheets of graphene [13].

In the fields of chemical graph theory, molecular topology and mathematical chemistry, a topological index, also known as a connectivity index is a type of molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph that characterize its topology, and they are usually graph-invariant. Topological indices are used, for example, in the development of quantitative structure-activity relationships in which the biological activity or other properties of molecules are correlated with their chemical structure. Wiener first used a topological index in science to investigate paraffin breaking points [26]; this was followed by other efforts to elucidate physico-chemical features, culminating in the presentation of a variety of topological descriptors. The authors of [27] put forward a new idea for degree-based topological indices, which they nambed "*ve*-degree and *ev*-degree". The interesting basics of this new idea are detailed in [28–31].

Many papers have been written and various studies have been performed on topological indices as a result of the wide range of applications of topological indices in biology and chemistry [32–34]. For a molecular structure, the edge-splitting approach was applied in [35]; honeycomb networks are discussed in [36,37]; a hexagon star network was developed in [38];a hex-derived network is described in [39]; interconnection system topological indices are discussed in [40]. In addition, some biological, chemical and other degree-based properties of structures are discussed in [41, 42]. The articles solely focused on the vertex-edge and edge-vertex topological indices are given here in detail. For some examples, [43] discusses some general graphs on this topic, titanium dioxide nanotubes are discussed with this idea of indices in [44], [45] focuses on some metal trihalides networks and the hexagon star network have been studied [46]. Structures devised by the generalizations of two graph operations and their topological descriptors detailed in [47], computation of edge- and vertex-degree-based topological indices for tetrahedral sheets of clay minerals found in [48]. Few studies on the edge-vertex- and vertex-edge-related topological indices are presented in [49–51]. Some new and linked topics are dicussed in [52–55].

With the exception of the examples given above, topological indices have other uses, particularly in chemistry [56, 57]. The main focus of this paper is on expanding the applicability of armchair carbon nanotubes ($ACNT\,(p,q)$) and investigating various degree-based topological indices for armchair carbon semi-capped nanotubes ($ACSCNT\,(p,q)$) and armchair carbon capped nanotubes ($ACCNT\,(p,q)$).

A graphical representation of an armchair carbon capped nanotube is shown in Figure 1. Figure 2 depicts a three-dimensional view of capped and semi-capped armchairs.

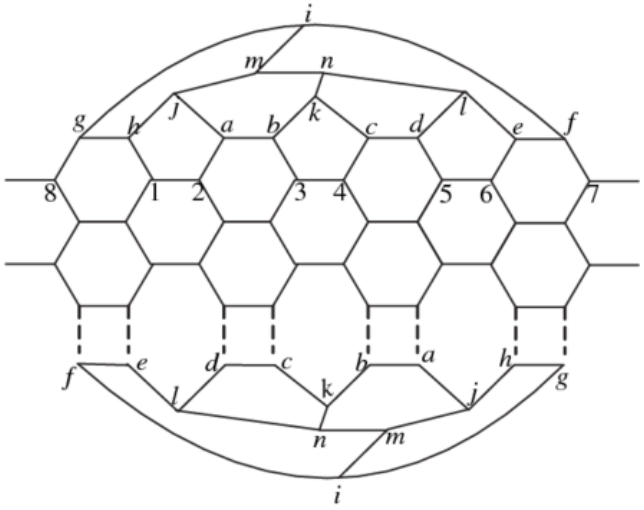

Figure 1. Illustration of armchair carbon $ACCNT\,(p,q)$.

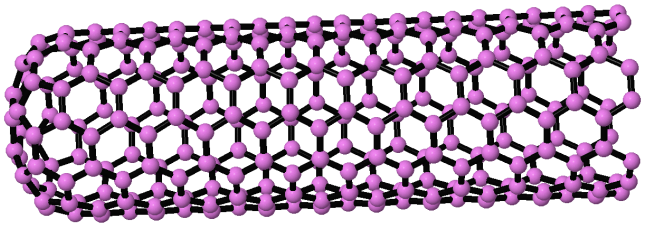

Figure 2. Semi-capped nanotube, $ACSCNT\,(p,q)$.

2. Preliminaries

A combination of V, which is referred to as a vertex set that is usually non-empty, and E, which is the edge set for vertices, is called a graph and denoted by $G = (V,E)$. Let say that the order and size or the number of members in the vertex and edge sets are denoted by x and y, respectively. The non-empty vertex set is transferred from atoms, and the edges are usually denoted by the bonds in a molecular graph. Let a notation $\Psi(\theta)$ be the count of edges attached to a vertex θ; this context is named as a degree of the θ-vertex. A graph can also be represented by a sequence of numbers or numerical quantities; sometimes, a matrix is also replaced by a graph. A numerical way of representing a graph is a topological index, and this context shows the different characterizations of the graph. There are many different types of topological indices, and they are distinguished by their methodologies. But, here, we will follow the method for degree-based topological indices, and it is very popular in fields ranging

from chemistry through chemical graph theory. Given below are some topological indices based on the degree relation of a graph that we implement to evaluate the main theorems in this paper.

The term $N(\theta)$ is called the open neighborhood degree of a vertex θ, and this concept is defined as the count of vertices attached to a θ-vertex. We take union of a vertex θ in the $N(\theta)$ set, which is defined as a closed neighborhood of the θ-vertex and labeled as $N[\theta]$. The ev-degree of any edge $e = \theta\vartheta \in E$ is labeled as $\Psi_{ev}(e)$ and defined as the total count of unions of the closed neighborhoods of vertices θ and ϑ. The ve-degree written is as $\Psi_{ve}(\theta)$ and defined for any vertex $\theta \in V$ by the total count of different edges that are attached to any closed neighborhood vertex of θ. The intense literature on this topic and clearly view of these definitions we refer to see [55]. Moreover, few of the topological indices for the above defined methods are formulated as below.

$$\mathbb{M}_{ev}(G) = \sum_{\vartheta \in E} \Psi_{ev}(\theta)^2, \tag{2.1}$$

$$\mathbb{M}^1_{\alpha ve}(G) = \sum_{\vartheta \in V} \Psi_{ve}(\vartheta)^2, \tag{2.2}$$

$$\mathbb{M}^1_{\beta ve}(G) = \sum_{\theta\vartheta \in E} (\Psi_{ve}(\theta) + \Psi_{ve}(\vartheta)), \tag{2.3}$$

$$\mathbb{M}^2_{ve}(G) = \sum_{\theta\vartheta \in E} (\Psi_{ve}(\theta) \times \Psi_{ve}(\vartheta)), \tag{2.4}$$

$$\mathbb{R}_{ve}(G) = \sum_{\theta\vartheta \in E} (\Psi_{ve}(\theta) \times \Psi_{ve}(\vartheta))^{-\frac{1}{2}}, \tag{2.5}$$

$$\mathbb{R}_{ev}(G) = \sum_{\vartheta E} \Psi_{ve}(\vartheta)^{-\frac{1}{2}}, \tag{2.6}$$

$$\mathbb{ABC}_{ve}(G) = \sum_{\theta\vartheta \in E} \left(\frac{\Psi_{ve}(\theta) + \Psi_{ve}(\vartheta) - 2}{\Psi_{ve}\theta \times \Psi_{ve}(\vartheta)} \right)^{\frac{1}{2}}, \tag{2.7}$$

$$\mathbb{GA}_{ve}(G) = \sum_{\theta\vartheta \in E} \frac{2(\Psi_{ve}(\theta) \times \Psi_{ve}(\vartheta))^{\frac{1}{2}}}{\Psi_{ve}(\theta) + \Psi_{ve}(\vartheta)}, \tag{2.8}$$

$$\mathbb{H}_{ve}(G) = \sum_{\theta\vartheta \in E} \frac{2}{\Psi_{ve}(\theta) + \Psi_{ve}(\vartheta)}, \tag{2.9}$$

$$\chi_{ve}(G) = \sum_{\theta\vartheta \in E} (\Psi_{ve}(\theta) + \Psi_{ve}(\vartheta))^{-\frac{1}{2}}. \tag{2.10}$$

The ev-degree Zagreb α index is defined in Eq (2.1); the first ve-degree Zagreb α index and first ve-degree Zagreb β index are defined in Eqs (2.2) and (2.3); the second ve-degree Zagreb index is described in the Eq (2.4); the ve- and ev-degree Randić indices are respectively defined in Eqs (2.5) and (2.6); the ve-degree atom-bond connectivity index is described by the Eq (2.7). Equation (2.8) presents the ve-degree geometric-arithmetic index, while Eqs (2.9) and (2.10) described the ve-degree harmonic index and ve-degree sum-connectivity index, respectively.

3. Results for $ACSCNT\,(p,q)$

Table 2 shows the different types of vertices by degree, while Tables 1 and 3 show that for edges; note that these specifications represent the semi-capped nanotubes made of carbon, i.e., $ACSCNT\,(p,q)$. In this section, we determine the *ev*-degree Zagreb index, first *ve*-degree Zagreb α/β index, second *ve*-degree Zagreb β index, *ve*-degree atom-bond connectivity ($\mathbb{ABC}_{ve}$) index, *ve*-degree geometric-arithmetic ($\mathbb{GA}_{ve}$) index, *ve*-degree Randic index, *ev*-degree Randic index, *ve*-degree sum-connectivity (χ_{ve}) index and *ve*-degree harmonic index ($\mathbb{H}_{ve}$) for semi-capped nanotubes made of carbon, i.e., $ACSCNT\,(p,q)$; note that, throughout the results we labeled this structural graph with $G_{p,q}$.

Table 1. *ev*-degree edge partition of a $G_{p,q}$ graph.

Number of edges	*ev*-degree	$(\Psi(\theta),\Psi(\vartheta))$
$\frac{p}{2}$	4	(2,2)
p	5	(2,3)
$\frac{3pq-4p}{2}$	6	(3,3)

Table 2. *ev*-degree vertex partition of a $G_{p,q}$ graph.

Number of vertices	*ve*-degree	$\Psi(\theta)$
p	5	2
p	8	3
$p(q-2)$	9	3

Table 3. *ev*-degree edge partition of a $G_{p,q}$ graph.

Number of edges	$(\Psi_{ve}(\theta),\Psi_{ve}(\vartheta))$	$(\Psi(\theta),\Psi(\vartheta))$
$\frac{p}{2}$	(5,5)	(2,2)
p	(5,8)	(2,3)
$\frac{p}{2}$	(8,8)	(3,3)
p	(8,9)	(3,3)
$\frac{3pq-7p}{2}$	(9,9)	(3,3)

3.1. *ev*-degree Zagreb index

The *ev*-degree Zagreb index can be computed by using Table 1, as follows:

$$M_{ev}\left(G_{p,q}\right)=\sum_{e_1\in E}\Psi_{ev}(e_1)^2,$$

$$= \left(\frac{p}{2}\right)(4)^2 + (p)(5)^2 + \left(\frac{3pq - 4p}{2}\right)(6)^2,$$
$$= 54pq - 39p.$$

3.2. First ve-degree Zagreb α index

The first *ve*-degree Zagreb α-index can be computed by using Table 2, as follows:

$$M^1_{\alpha ve}\left(G_{p,q}\right) = \sum_{x_1 \in V} \Psi_{ve}(x_1)^2,$$
$$= (p)(5)^2 + (p)(8)^2 + p(q-2)(9)^2,$$
$$= 81pq - 73p.$$

3.3. First ve-degree Zagreb β index

The first *ve*-degree Zagreb β index can be determined by using Table 3, follows:

$$M^1_{\beta ve}\left(G_{p,q}\right) = \sum_{\theta\vartheta \in E} \left(\Psi_{ve}(\theta) + \Psi_{ve}(\vartheta)\right),$$
$$= \frac{p}{2} \times (5+5) + p \times (5+8) + \frac{p}{2} \times (8+8) + p \times (8+9) + \frac{3pq - 7p}{2} \times (9+9),$$
$$= 27pq - 20p.$$

3.4. Second ve-degree Zagreb index

The second *ve*-degree Zagreb index can be calculated by using Table 3, as follows:

$$M^2_{ve}\left(G_{p,q}\right) = \sum_{\theta\vartheta \in E} \left(\Psi_{ve}(\theta) \times \Psi_{ve}(\vartheta)\right),$$
$$= \frac{p}{2} \times (5 \times 5) + p \times (5 \times 8) + \frac{p}{2} \times (8 \times 8) + p \times (8 \times 9) + \frac{3pq - 7p}{2} \times (9 \times 9),$$
$$= \frac{243\,pq}{2} - 127\,p.$$

3.5. ve-degree Randic index

The *ve*-degree Randić index can be calculated by using Table 3, as follows:

$$R_{ve}\left(G_{p,q}\right) = \sum_{\theta\vartheta \in E} \left(\Psi_{ve}(\theta) \times \Psi_{ve}(\theta)\right)^{-\frac{1}{2}},$$
$$= \frac{p}{2} \times (5 \times 5)^{-\frac{1}{2}} + p \times (5 \times 8)^{-\frac{1}{2}} + \frac{p}{2} \times (8 \times 8)^{-\frac{1}{2}} + p \times (8 \times 9)^{-\frac{1}{2}} + \frac{3pq - 7p}{2} \times (9 \times 9)^{-\frac{1}{2}},$$
$$= \frac{pq}{6} + \left(-\frac{163}{720} + 1/20\ \sqrt{10} + 1/12\ \sqrt{2}\right)p.$$

3.6. ve-degree atom-bond connectivity index

The *ve*-degree atom-bond connectivity index can be determined by using the values in Table 3, as follows:

$$\begin{aligned} ABC_{ve}\left(G_{p,q}\right) &= \sum_{\theta\vartheta\in E}\left(\frac{\Psi_{ve}(\theta)+\Psi_{ve}(\vartheta)-2}{\Psi_{ve}(\theta)\times\Psi_{ve}(\vartheta)}\right)^{\frac{1}{2}}, \\ &= \frac{p}{2}\times\sqrt{\frac{8}{25}}+p\times\sqrt{\frac{11}{40}}+\frac{p}{2}\times\sqrt{\frac{14}{64}}+p\times\sqrt{\frac{15}{72}}+\frac{3pq-7p}{2}\times\sqrt{\frac{16}{81}}, \\ &= \left(1/5\ \sqrt{2}+1/20\ \sqrt{110}+1/16\ \sqrt{14}+1/12\ \sqrt{30}-\frac{14}{9}\right)p+2/3\,pq. \end{aligned}$$

3.7. ve-degree geometric-arithmetic index

The *ve*-degree geometric-arithmetic index can be calculated by using the values defined in Table 3, as follows:

$$\begin{aligned} GA_{ve}\left(G_{p,q}\right) &= \sum_{\theta\vartheta\in E}\frac{2\left(\Psi_{ve}(\theta)\times\Psi_{ve}(\vartheta)\right)^{\frac{1}{2}}}{\Psi_{ve}(\theta)+\Psi_{ve}(\vartheta)}, \\ &= \frac{p\ \sqrt{25}}{10}+\frac{2p\ \sqrt{40}}{13}+\frac{p\ \sqrt{64}}{16}+\frac{2p\ \sqrt{72}}{17}+\frac{(3pq-7p)\ \sqrt{81}}{18}, \\ &= -5/2\,p+\frac{4\,p\sqrt{10}}{13}+\frac{12\,p\sqrt{2}}{17}+3/2\,pq. \end{aligned}$$

3.8. ve-degree harmonic index

The *ve*-degree harmonic index can be determined by using the values defined in Table 3, as follows:

$$\begin{aligned} H_{ve}\left(G_{p,q}\right) &= \sum_{\theta\vartheta\in E}\frac{2}{\Psi_{ve}(\theta)+\Psi_{ve}(\vartheta)}, \\ &= \frac{p}{10}+\frac{2p}{13}+\frac{p}{16}+\frac{2p}{17}+\frac{3pq-7p}{18}, \\ &= \frac{7177\,p}{159120}+pq/6. \end{aligned}$$

3.9. ve-degree sum-connectivity index

The *ve*-degree sum-connectivity index can be determined by using the values in Table 3, as follows:

$$\begin{aligned} \chi_{ve}\left(G_{p,q}\right) &= \sum_{\theta\vartheta\in E}\left(\Psi_{ve}(\theta)+\Psi_{ve}(\vartheta)\right)^{-\frac{1}{2}}, \\ &= \frac{p}{2}(10)^{-\frac{1}{2}}+p\,(13)^{-\frac{1}{2}}+\frac{p}{2}(16)^{-\frac{1}{2}}+\frac{p}{2}(17)^{-\frac{1}{2}}+\frac{3pq-7p}{2}(18)^{-\frac{1}{2}}, \\ &= 1/20\,p\sqrt{10}+1/13\,p\sqrt{13}+p/8+1/17\,p\sqrt{17}+1/12\ (3\,pq-7\,p)\ \sqrt{2}. \end{aligned}$$

4. Conclusions and discussion

The numerical values of all of the above-mentioned parameters, i.e., M_{ev}, $M^1_{\alpha ve}$, $M^1_{\beta ve}$, M^2_{ve}, R_{ve}, ABC_{ve}, GA_{ve}, H_{ve} and χ_{ve}, are defined in Tables 4 and 5. We present these results graphically in Figures 3 and 4.

Table 4. Numerical comparison of M_{ev}, $M^1_{\alpha ve}$, $M^1_{\beta ve}$, M^2_{ve} and R_{ve}.

[p,q]	M_{ev}	$M^1_{\alpha ve}$	$M^1_{\beta ve}$	M^2_{ve}	R_{ve}
[5, 5]	1155	1660	575	$\frac{4805}{2}$	4.4146
[6, 6]	1710	2478	852	3612	6.2975
[7, 7]	2373	3458	1183	$\frac{10129}{2}$	8.5136
[8, 8]	3144	4600	1568	6760	11.063
[9, 9]	4023	5904	2007	$\frac{17397}{2}$	13.946
[10, 10]	5010	7370	2500	10880	17.162
[11, 11]	6105	8998	3047	$\frac{26609}{2}$	20.711
[12, 12]	7308	10788	3648	15972	24.594
[13, 13]	8619	12740	4303	$\frac{37765}{2}$	28.812
[14, 14]	10038	14854	5012	22036	33.361

Table 5. Numerical comparison of ABC_{ve}, GA_{ve}, H_{ve} and χ_{ve}.

[p,q]	H_{ve}	ABC_{ve}	GA_{ve}	χ_{ve}
[5, 5]	16.377	34.856	4.3922	8.7291
[6, 6]	23.652	50.828	6.2706	12.596
[7, 7]	32.261	69.799	8.4824	17.170
[8, 8]	42.202	91.770	11.028	22.451
[9, 9]	53.478	116.74	13.906	28.440
[10, 10]	66.086	144.71	17.118	35.136
[11, 11]	80.029	175.68	20.663	42.538
[12, 12]	95.303	209.66	24.541	50.648
[13, 13]	111.91	246.63	28.753	59.465
[14, 14]	129.86	286.60	33.298	68.988

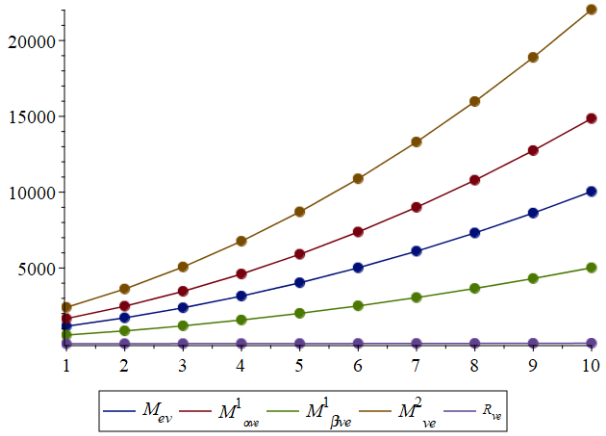

Figure 3. Graphical comparison of M_{ev}, $M^1_{\alpha ve}$, $M^1_{\beta ve}$, M^2_{ve} and R_{ve} for $G_{p,q}$.

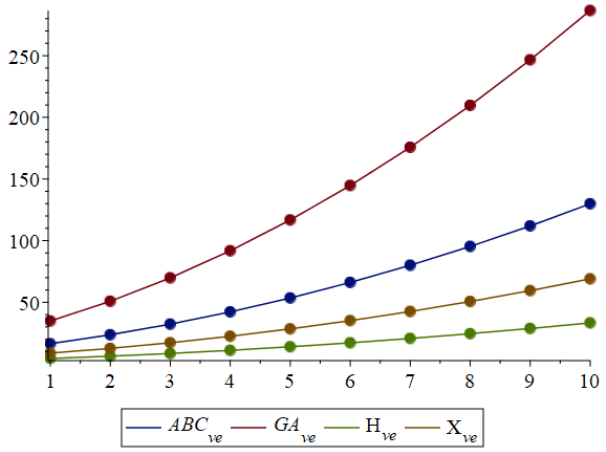

Figure 4. Graphical comparison of ABC_{ve}, GA_{ve}, H_{ve} and χ_{ve} for $G_{p,q}$.

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Conflict of interest

The authors declare that there is no conflict of interest.

References

1. S. Iijima, Helical microtubules of graphitic carbon, *Nature*, **354** (1991), 56–58. https://doi.org/10.1038/354056a0

2. M. F. Thorpe, D. Tománek, R. J. Enbody, *Science and Application of Nanotubes*, Springer, 2002.
3. U. Kuhlmann, H. Jantoljak, N. Pfander, P. Bernier, C. Journet, C. Thomsen, Infrared active phonons in single-walled carbon nanotubes, *Chem. Phys. Lett.*, **294** (1998), 237–240. https://doi.org/10.1016/S0009-2614(98)00845-8
4. P. Mlynarska, S. Tomczewski, A. Pakuła, G. Wróblewski, M. Sloma, L. Salbut, Detection of subsurface defects and measurement of thickness of screen layers made of graphene and carbon nanotubes with application of full-field optical coherence tomography in linnik configuration, in *Optical Manufacturing and Testing XI*, **9575** (2015), 246–251. https://doi.org/10.1117/12.2188640
5. J. Tang, Y. Wang, S. Cheng, P. Yu, K. Huang, C. Yuan, Applications of single-walled carbon nanotubes and type-II quantum dots in photovoltaics and passive mode-locking saturable absorbers, in *Carbon Nanotubes, Graphene, and Associated Devices V*, **8462** (2012), 108–119. https://doi.org/10.1117/12.928211
6. P. Li, W. Xue, Dielectrophoretic assembly of organized carbon nanotubes and thin films, in *ASME International Mechanical Engineering Congress and Exposition*, **44496** (2010), 49–54. https://doi.org/10.1115/IMECE2010-37441
7. R. P. Raffaelle, B. Landi, T. Gennett, R. S. Morris, B. Dixon, P. Lamarre, Fuel cell applications of single wall carbon nanotubes, in *International Conference on Fuel Cell Science, Engineering and Technology*, **36681** (2003), 121–128. https://doi.org/10.1115/FUELCELL2003-1708
8. S. A. Bakar, S. Muhamad, A. A. Aziz, N. A. Asli, M. Mohammad, M. S. Shamsudin, et al., CVD growth of carbon nanotubes from palm oil precursor, in *2012 IEEE Symposium on Business, Engineering and Industrial Applications*, IEEE, (2012), 377–381. https://doi.org/10.1109/ISBEIA.2012.6422908
9. E. V. Antoniadou, B. G. Cousins, A. M. Seifalian, Development of conductive polymer with carbon nanotubes for regenerative medicine applications, in *2010 Annual International Conference of the IEEE Engineering in Medicine and Biology*, IEEE, (2010), 815–818. https://doi.org/10.1109/IEMBS.2010.5626760
10. R. Sen, T. Kocab, J. Black, J. McDermott, S. K. Pal, S. Buffat, et al., Engineering nanomaterials and nanostructures for electronic applications: A case study of carbon nanotubes for memory devices, in *2020 4th IEEE Electron Devices Technology & Manufacturing Conference (EDTM)*, IEEE, (2020). https://doi.org/10.1109/EDTM47692.2020.9117911
11. C. A. C. Abdullah, E. L. Albert, Carbon nanotubes as biological transporters and tissue-engineering scaffolds, in *Synthesis, Technology and Applications of Carbon Nanomaterials*, Elsevier, (2019), 135–156. https://doi.org/10.1016/B978-0-12-815757-2.00006-1
12. N. Mamidi, Cytotoxicity evaluation of carbon nanotubes for biomedical and tissue engineering applications, in *Perspective of Carbon Nanotubes*, IntechOpen, 2019.
13. M. K. Assadi, H. Hanaei, Transparent carbon nanotubes (CNTs) as antireflection and self-cleaning solar cell coating, in *Engineering Applications of Nanotechnology*, Springer, Cham, (2017), 101–114. https://doi.org/10.1007/978-3-319-29761-3_4
14. P. J. Britto, K. S. V. Santhanam, A. Rubio, J. A. Alonso, P. M. Ajayan, Improved charge transfer at carbon nanotube electrodes, *Adv. Mater.*, **11** (1999), 154–157. https://doi.org/10.1002/(SICI)1521-4095(199902)11:2<154::AID-ADMA154>3.0.CO;2-B

15. G. A. Rivas, M. D. Rubianes, M. C. Rodríguez, N. F. Ferreyra, G. L. Luque, M. L. Pedano, et al., Carbon nanotubes for electrochemical biosensing, *Talanta*, **74** (2007), 291–307. https://doi.org/10.1016/j.talanta.2007.10.013

16. A. J. S. Ahammad, J. J. Lee, Md. A. Rahman, Electrochemical sensors based on carbon nanotubes, *Sensors*, **9** (2009), 2289–2319. https://doi.org/10.3390/s90402289

17. A. N. Ribeiro, N. S. Ferreira. Systematic study of the physical origin of ferromagnetism in CeO2-nanoparticles, *Phys. Rev. B*, **95** (2017), 144430. https://doi.org/10.1103/PhysRevB.95.144430

18. E. N. Tseng, Y. T. Hsiao, Y. C. Chen, S. Y. Chen, A. Gloter, J. M. Song, Magnetism and plasmonic performance of mesoscopic hollow ceria spheres decorated with silver nanoparticles, *Nanoscale*, **11** (2019), 3574–3582. https://doi.org/10.1039/C8NR09636H

19. S. A. Holgate, *Understanding Solid State Physics*, CRC Press, 2009.

20. H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley, C60: Buckminsterfullerene, *Nature*, **318** (1985), 162–163. https://doi.org/10.1038/318162a0

21. A. Younis, D. Chu, S. Li, Cerium oxide nanostructures and their applications, in *Functionalized Nanomaterials*, InTech, 2016.

22. S. T. R. Naqvi, B. Shirinfar, S. Majeed, M. N. Haq, D. Hussain, T. Iqbal, et al., Synthesis, design and sensing applications of nanostructured ceria-based materials, *Analyst.*, **143** (2018), 5610–5628. https://doi.org/10.1039/c8an01268g

23. A. Dhall, W. Self, Cerium oxide nanoparticles: A brief review of their synthesis methods and biomedical applications, *Antioxidants*, **7** (2018), 97. https://doi.org/10.3390/antiox7080097

24. S. Borgmann, A. Schulte, S. Neugebauer, W. Schuhmann, Amperometric biosensors, in *Advances in Electrochemical Sciences and Engineering*, (2012), 1–83.

25. E. N. Primo, F. Gutiérrez, M. D. Rubianes, N. F. Ferreyra, M. C. Rodríguez, M. L. Pedano, et al., Electrochemistry in one dimension: Applications of carbon nanotubes, in *Advances in Electrochemical Sciences and Engineering*, **2015** (2015), 83–120. https://doi.org/10.1002/9783527697489.ch3

26. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.*, **69** (1947), 17–20. https://doi.org/10.1021/ja01193a005

27. S. B. Chen, A. Rauf, M. Ishtiaq, M. Naeem, A. Aslam, On ve-degree- and ev-degree-based topological properties of crystallographic structure of cuprite Cu2o, *Open Chem.*, **19** (2021), 576–5851. https://doi.org/10.1515/chem-2021-0051

28. S. Ediz, A new tool for QSPR researches: ev-degree randić index, *Celal Bayar Univ. J. Sci.*, **13** (2017), 615–618. https://doi.org/10.1177/1559827617729634

29. S. Ediz, On ve-degree molecular topological properties of silicate and oxygen networks, *Int. J. Comput. Sci. Math.*, **9** (2018). https://doi.org/10.1504/ijcsm.2018.10011733

30. B. Sahin, S. Ediz, On ev-degree and ve-degree topological indices, *Iran. J. Math. Chem.*, **9** (2018).

31. M. Chellali, T. W. Haynes, S. T. Hedetniemi, T. M. Lewis, On ve-degrees and ev-degrees in graphs, *Discrete Math.*, **340** (2007), 31–38. https://doi.org/10.4028/www.scientific.net/KEM.340-341.31

32. M. F. Nadeem, M. Azeem, I. Farman, Comparative study of topological indices for capped and uncapped carbon nanotubes, *Polycyclic Aromat. Compd.*, **2021** (2021), 1–18. https://doi.org/10.1080/10406638.2021.1903952

33. M. F. Nadeem, M. Azeem, H. M. A.Siddiqui, Comparative study of zagreb indices for capped, semi-capped, and uncapped carbon nanotubes, *Polycyclic Aromat. Compd.*, **2021** (2021), 1–18. https://doi.org/10.1080/10406638.2021.1890625

34. M. F. Nadeem, M. Imran, H. M. A. Siddiqui, M. Azeem, A. Khalil, Y. Ali, Topological aspects of metal-organic structure with the help of underlying networks, *Arabian J. Chem.*, **14** (2021), 103157. https://doi.org/10.1016/j.arabjc.2021.103157

35. W. Gao, M. R. Farahani, Degree-based indices computation for special chemical molecular structures using edge dividing method, *Appl. Math. Nonlinear Sci.*, **1** (2016), 99–122. https://doi.org/10.21042/AMNS.2016.1.00009

36. S. Hayat, M. A. Malik, M. Imran, Computing topological indices of honeycomb derived networks, *Rom. J. Inf. Sci. Technol.*, **18** (2015), 144–165. https://doi.org/10.1525/nr.2015.18.3.144

37. A. Ahmad, Computation of certain topological properties of para-line graph of honeycomb networks and graphene, *Discrete Math. Algorithms Appl.*, **9** (2017), 1750064. https://doi.org/10.1142/S1793830917500641

38. A. N. A. Koam, A. Ahmad, M. F. Nadeem, Comparative study of valency-based topological descriptor for hexagon star network, *Comput. Syst. Sci. Eng.*, **36** (2021), 293–306. https://doi.org/10.32604/csse.2021.014896

39. A. N. A. Koam, A. Ahmad, A. A. H. Ahmadini, Computation of vertex-edge degree based topological descriptors for hex-derived network, *IEEE Access*, **9** (2021), 82989–83001. https://doi.org/10.1109/ACCESS.2021.3086451

40. A. Ahmad, R. Hasni, K. Elahi, M. A. Asim, Polynomials of degree-based indices for swapped networks modeled by optical transpose interconnection system, *IEEE Access*, **8** (2020), 214293–214299. https://doi.org/10.1109/ACCESS.2020.3039298

41. A. Shabbir, M. F. Nadeem, S. Mukhtar, A. Raza, On edge version of some degree-based topological indices of HAC5c7 [p,q] and VC5c7[p,q] nanotubes, *Polycyclic Aromat. Compd.*, (2020), 1–17. https://doi.org/10.1080/10406638.2020.1753220

42. N. Zahra, M. Ibrahim, M. K. Siddiqui, On topological indices for swapped networks modeled by optical transpose interconnection system, *IEEE Access*, **8** (2020), 200091–200099. https://doi.org/10.1109/ACCESS.2020.3034439

43. B. Horoldagva, K. C. Das, T. A. Selenge, On ve-degree and ev-degree of graphs, *Discrete Optim.*, **31** (2019), 1–7. https://doi.org/10.1016/j.disopt.2018.07.002

44. J. Zhang, M. K. Siddiqui, A. Rauf, M. Ishtiaq, On ve-degree and ev-degree based topological properties of single walled titanium dioxide nanotube, *J. Cluster Sci.*, **32** (2020), 821–832. https://doi.org/10.1007/s10876-020-01842-3

45. F. A. Abolaban, A. Ahmad, M. A. Asim, Computation of vertex-edge degree based topological descriptors for metal trihalides network, *IEEE Access*, **9** (2021), 65330–65339. https://doi.org/10.1109/ACCESS.2021.3076036

46. E. A. Refaee, A. Ahmad, A study of hexagon star network with vertex-edge-based topological descriptors, *Complexity*, **2021** (2021), 9911308. https://doi.org/10.1155/2021/9911308
47. H. Raza, M. Waheed, M. K. Jamil, M. Azeem, Structures devised by the generalizations of two graph operations and their topological descriptors, *Main Group Met. Chem.*, **45** (2022), 44–56. https://doi.org/10.1515/mgmc-2022-0006
48. A. N. A. H. Ahmad, A. Ahmad, M. Azeem, Computation of edge- and vertex-degree-based topological indices for tetrahedral sheets of clay minerals, *Main Group Met. Chem.*, **45** (2022), 26–34. https://doi.org/10.1515/mgmc-2022-0007
49. A. Ahmad, Vertex-degree based eccentric topological descriptors of zero divisor graph of commutative rings, *Online J. Anal. Comb.*, **15** (2020), 1–10.
50. A. Ahmad, On the degree based topological indices of benzene ring embedded in p-type-surface in 2d network, *Hacettepe J. Math. Stat.*, **47** (2018), 9–18.
51. A. Ahmad, K. Elahi, R. Hasni, M. F. Nadeem, Computing the degree based topological indices of line graph of benzene ring embedded in p-type-surface in 2d network, *J. Inf. Optim. Sci.*, **40** (2019), 1511–1528. https://doi.org/10.1017/S0144686X19000138
52. A. N. A. Koam, A. Ahmad, M. A. Asim, M. Azeem, Computation of vertex and edge resolvability of benzenoid tripod structure, *J. King Saud Univ. Sci.*, **34** (2022), 102208. https://doi.org/10.1016/j.jksus.2022.102208
53. A. N. A. Koam, A. Ahmad, M. Azeem, A. Khalil, M. F. Nadeem, On adjacency metric dimension of some families of graph, *J. Funct. Spaces*, **2022** (2022), 6906316. https://doi.org/10.1155/2022/6906316
54. S. Hameed, M. K. Jamil, M. Waheed, M. Azeem, S. Swaray, Two complex graph operations and their exact formulations on topological properties, *Complexity*, **2022** (2022), 1–15. https://doi.org/10.1155/2022/6331366
55. M. Azeem, M. Imran, M. F. Nadeem, Sharp bounds on partition dimension of hexagonal möbius ladder, *J. King Saud Univ. Sci.*, **34** (2022), 101779. https://doi.org/10.1016/j.jksus.2021.101779
56. W. Wu, C. Zhang, W. Lin, Q. Chen, X. Guo, Y. Qian, et al., Quantitative structure-property relationship (QSPR) modeling of drug-loaded polymeric micelles via genetic function approximation, *PLOS One*, **10** (2015), e0119575. https://doi.org/10.1371/journal.pone.0119575
57. X. Zhang, A. Raza, A. Fahad, M. K. Jamil, M. A. Chaudhry, Z. Iqbal, On face index of silicon carbides, *Discrete Dyn. Nat. Soc.*, **2020** (2020), 6048438. https://doi.org/10.1155/2020/6048438

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