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Computation of General Zagreb Index of Nanotubes Covered by C_5 and C_7

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Abstract: A molecular graph is hydrogen deleted simple connected graph in which vertices and edges are represented by atoms and chemical bonds, respectively. Topological indices are numerical parameters of a molecular graph which characterize its topology and are usually graph invariant. In Mathematical chemistry, topological descriptors play an important role in modeling different physical and chemical activities of molecules. In this study, the generalized Zagreb index for three types of carbon nanotubes is computed. By putting some particular values to the parameters, some important degree-based topological indices are also derived.

Keywords: Molecular graph; degree; topological index; generalized Zagreb index; carbon nanotube.

1. Introduction

Throughout this article, we consider only a simple connected graph. Let $G = \left(V(G), E(G)\right)$ be a graph with $V(G)$ and $E(G)$ as vertex and edge sets, respectively. The degree of a vertex $v \in V(G)$is denoted by $d_G(v)$, is the total count of nodes connected to v in G. Mathematical Chemistry is a topic of inquiry in chemistry wherein mathematical tools are often used to deal with the issues of chemistry. Chemical graph theory is an active research area in mathematical chemistry that interacts with the topology of chemical composition, such as the mathematical study of isomerism and the advancement of topological indices. A topological index is a real number obtained from the graph mathematically or, more generally, a molecular descriptor that allows us to understand some of the physical and chemical properties of molecules. Lots of topological indices have been designed in the literature. The present work deals with the degree-based topological indices of carbon nanotubes. The first degree based indices are the Zagreb indices introduced by Gutman and Trinajestic′ [1] to investigate the total π–electron energy of carbon atoms. They are formulated as follows:

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

and

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

The forgotten topological index or F-index was introduced by Furtula and Gutman in 2015 [2]. It was formulated as,

$$F(G)=\sum_{v\in V(G)} d_G(v)^3=\sum_{uv\in E(G)}[d_G(u)^2+d_G(v)^2].$$

Ranjini *et al.* in [3] introduced following redefined Zagreb index in 2013

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

Li and Zheng [4] presented the idea of the general Zagreb index which is defined as

$$M^\alpha(G)=\sum_{u\in V(G)} d_G(u)^\alpha$$

where, $\alpha\neq 0,1, and\ \alpha\in\mathbb{R}$. Thus, $\alpha=2$ produces the first Zagreb index, and $\alpha=3$ yields the F-index. Gutman and Lepovic$'$, first generalized the Randic$'$ index in 2001 [5] and is defined as

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

where,$\alpha\neq 0,\ \alpha\in\mathbb{R}$.

The Symmetric division deg index of a graph is formulated as

$$SDD(G)=\sum_{uv\in E(G)}[\frac{d_G(u)}{d_G(v)}+\frac{d_G(v)}{d_G(u)}].$$

For more discussion about it, readers are referred to [6-8]. Azari *et al.* in [9] presented a generalized degree-based topological index, known as generalized Zagreb index or the (a,b) −Zagreb index and is defined as follows:

$$Z_{(a,b)}(G)=\sum_{uv\in E(G)}[d_G(u)^a d_G(v)^b+d_G(u)^b d_G(v)^a].$$

The relationship between (a,b) −Zagreb index and different particular degree-based indices are shown in Table 1.

Table 1. Relations between (a,b)-Zagreb index with some other topological indices.

Topological index	Corresponding generalized Zagreb index
$\boldsymbol{M_1(G)}$	$Z_{(1,0)}(G)$
$\boldsymbol{M_2(G)}$	$\frac{1}{2}Z_{(1,1)}(G)$
F(G)	$Z_{(2,0)}(G)$
ReZM(G)	$Z_{(2,1)}(G)$
$\boldsymbol{M^\alpha(G)}$	$Z_{(\alpha-1,0)}(G)$
$\boldsymbol{R_\alpha(G)}$	$\frac{1}{2}Z_{(\alpha,\alpha)}(G)$
SDD(G)	$Z_{(1,-1)}(G)$

A nanostructure is an intermediate object between microscopic and molecular structures. It is a molecular-scale product obtained from engineering. Nanotubes are very good thermal conductors and are an ideal material for applications in electronics and optics. The most important class of such materials is carbon nanotubes. Carbon nanotubes are carbon allotropes with cylindrical molecular structures, having diameters ranging from a few nanometers and lengths to several millimeters. The present work deals with the nanotubes covered by C_5 and C_7. Hayat and Imran [10] obtained some degree based indices of $VC_5C_7[p,q]$, $HC_5C_7[p,q]$, and $SC_5C_7[p,q]$. Mondal *et al.* [11] calculated topological indices of some nanostructures. Farahani [12] derived the generalized Zagreb index of circumcoronene series of benzenoid. Sardar *et al.* [13] computed the generalized Zagreb index of the structure of the Capra-designed planar benzenoid series. For more works on this field, readers are referred to [14-22].

2. Materials and Methods

Our main results include degree-based topological indices of three types of carbon nanotubes. Firstly we obtain the generalized Zagreb index, and then by putting some particular values to the parameters, some important degree-based topological indices are computed. To compute the outcomes, it was used the method of combinatorial computing, vertex partition method, edge partition method, graph-theoretical tools, analytic techniques, and degree counting method.

3. Results and Discussion

The present section deals with the derivation of (a,b)-Zagreb index for some nanotubes covered by C_5 and C_7. We start with the nanotube $VC_5C_7[p,q]$. The two-dimensional structure of $VC_5C_7[p,q]$ is depicted in Figure 1. Its edge partition is shown in Table 2.

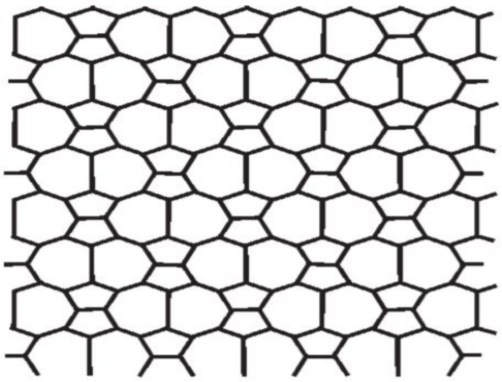

Figure 1. The graph of $VC_5C_7[p,q]$ nanotube with $p = 3$ and $q = 4$.

Table 2. Edge partition of $VC_5C_7[p,q]$ nanotubes based on degrees of end vertices of each edge.

$(\mathbf{d(u)}, \mathbf{d(v)})$, $\mathbf{uv} \in \boldsymbol{E(G)}$	**Number of edges**
(2,2)	*P*
(2,3)	*10p*
(3,3)	*24pq-14p*

$$E_1(VC_5C_7[p,q]) = \{uv \in E(VC_5C_7[p,q]): d(u) = 2, d(v) = 2\},$$
$$E_2(VC_5C_7[p,q]) = \{uv \in E(VC_5C_7[p,q]): d(u) = 2, d(v) = 3\},$$
$$E_3(VC_5C_7[p,q]) = \{uv \in E(VC_5C_7[p,q]): d(u) = 3, d(v) = 3\}.$$

Theorem 1. The (a,b) −Zagreb index of $VC_5C_7[p,q]$ is given by

$$Z_{(a,b)}(VC_5C_7[p,q]) = p.2^{a+b+1} + 10p(2^a3^b + 2^b3^a) + 4p(12q-7)3^{(a+b)}.$$

Proof. Applying the definition of general Zagreb index, we have from Table 1, 2,

$$Z_{(a,b)}(VC_5C_7[p,q]) = \sum_{uv\in E(VC_5C_7[p,q])} (d(u)^a d(v)^b + d(u)^b d(v)^a)$$
$$= \sum_{uv\in E_1(VC_5C_7[p,q])} (d(u)^a d(v)^b + d(u)^b d(v)^a)$$
$$+ \sum_{uv\in 2(VC_5C_7[p,q])} (d(u)^a d(v)^b + d(u)^b d(v)^a)$$

$$+\sum_{uv\in E_3(VC_5C_7[p,q])}(d(u)^a d(v)^b + d(u)^b d(v)^a)$$
$$= |E_1(VC_5C_7[p,q])|\,(2^a2^b + 2^b2^a)$$
$$+|E_2(VC_5C_7[p,q])|\,(2^a3^b + 2^b3^a)$$
$$+|E_3(VC_5C_7[p,q])|\,(3^a3^b + 3^b3^a)$$
$$= p.2.2^{a+b} + 10p(2^a3^b + 2^b3^a) + (24pq - 14p).2.3^{(a+b)}$$
$$= p.2^{a+b+1} + 10p(2^a3^b + 2^b3^a) + 4p(12q - 7)3^{(a+b)}.$$

Hence, the theorem. □

Corollary 1. Using Theorem 1, we have the following results:

(i) $M_1(G) = Z_{1,0}(G) = 144pq - 30p,$

(ii) $M_2(G) = \frac{1}{2}Z_{1,1}(G) = 432pq - 124p,$

(iii) $F(G) = Z_{2,0}(G) = 432pq - 114p,$

(iv) $ReZM(VC_5C_7[p,q]) = Z_{(2,1)}(VC_5C_7[p,q]) = 1296pq - 440p,$

(v) $SDD(VC_5C_7[p,q]) = Z_{(1,-1)}(VC_5C_7[p,q]) = 4pq - \frac{13}{3}p.$

Theorem 2. The (a,b) −Zagreb index of $HC_5C_7[p,q]$ is given by

$$Z_{(a,b)}(HC_5C_7[p,q]) = 8p(2^a3^b + 2^b3^a) + 4p(12q - 5)3^{(a+b)}.$$

Proof. The two-dimensional structure of $HC_5C_7[p,q]$ is shown in Figure 2. Its edge partition is shown in Table 3.

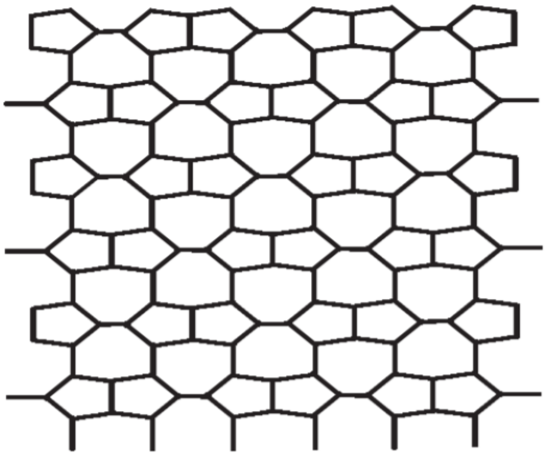

Figure 2. The graph of $HC_5C_7[p,q]$ nanotube with $p = 3$ and $q = 3$.

Table 3. Edge partition of $HC_5C_7[p,q]$ nanotubes based on degrees of end vertices of each edge.

$(\mathbf{d(u)}, \mathbf{d(v)})$, $\mathbf{uv} \in \boldsymbol{E(G)}$	**Number of edges**
(2,3)	10p
(3,3)	24pq-14p

$$E_1(HC_5C_7[p,q]) = \{uv \in E(VC_5C_7[p,q]): d(u) = 2, d(v) = 3\},$$
$$E_2(HC_5C_7[p,q]) = \{uv \in E(VC_5C_7[p,q]): d(u) = 3, d(v) = 3\}$$

Using the definition of general Zagreb index, we have from Table 1, 3,

$$Z_{(a,b)}(HC_5C_7[p,q]) = \sum_{uv\in E(HC_5C_7[p,q])}(d(u)^a d(v)^b + d(u)^b d(v)^a)$$
$$= \sum_{uv\in E_1(HC_5C_7[p,q])}(d(u)^a d(v)^b + d(u)^b d(v)^a)$$

$$+\sum_{uv\in 2(HC_5C_7[p,q])}(d(u)^a d(v)^b + d(u)^b d(v)^a)$$
$$= |E_1(HC_5C_7[p,q])|\,(2^a3^b + 2^b3^a)$$
$$+|E_2(HC_5C_7[p,q])|\,(3^a3^b + 3^b3^a)$$
$$= 8p(2^a3^b + 2^b3^a) + (24pq - 10p).2.3^{(a+b)}$$
$$= 8p(2^a3^b + 2^b3^a) + 4p(12q - 5)3^{(a+b)}.$$

Hence, the theorem. □

Corollary 2. From Theorem 2, we have the following results:

(i) $M_1(HC_5C_7[p,q]) = Z_{1,0}(HC_5C_7[p,q]) = 144pq - 20p,$

(ii) $M_2(HC_5C_7[p,q]) \quad = \frac{1}{2}Z_{1,1}(HC_5C_7[p,q]) = 216pq - 42p,$

(iii) $F(HC_5C_7[p,q]) \quad = Z_{2,0}(HC_5C_7[p,q]) = 432pq - 76p,$

(iv) $ReZM(HC_5C_7[p,q]) = Z_{(2,1)}(HC_5C_7[p,q]) = 1296pq - 300p,$

(v) $SDD(HC_5C_7[p,q]) = Z_{(1,-1)}(HC_5C_7[p,q]) = 48pq - \frac{8}{3}p,$

(vi) $R_\alpha(HC_5C_7[p,q]) \quad = \frac{1}{2}Z_{(\alpha,\alpha)}(HC_5C_7[p,q]) = 24pq^{\alpha+1} + 8p.6^\alpha - 10p.q^\alpha,$

(vii) $M^\alpha(HC_5C_7[p,q]) = Z_{(\alpha-1,0)}(HC_5C_7[p,q]) = 8p.2^{\alpha-1} - 12p.3^{\alpha-1} - 48pq.3^{\alpha-1}.$

Theorem 3. The (a,b) −Zagreb index of $SC_5C_7[p,q]$ is given by

$$Z_{(a,b)}(SC_5C_7[p,q]) = p.2^{a+b+1} + 6p(2^a3^b + 2^b3^a) + 6p(4q-3).3^{(a+b)}.$$

Proof. The two-dimensional structure of $SC_5C_7[p,q]$ is depicted in Figure 3. Its edge partition is shown in Table 4.

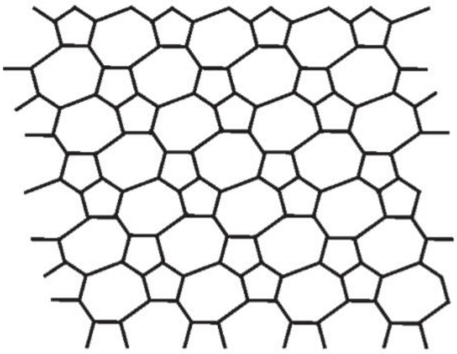

Figure 3. The graph of $SC_5C_7[p,q]$ nanotube with $p = 4$ and $q = 4$.

Table 4. Edge partition of $SC_5C_7[p,q]$ nanotubes based on degrees of end vertices of each edge.

$(\mathbf{d(u)}, \mathbf{d(v)})$, $\mathbf{uv} \in \boldsymbol{E(G)}$	**Number of edges**
(2,2)	P
(2,3)	6p
(3,3)	12pq-9p

$$E_1(SC_5C_7[p,q]) = \{uv \in E(SC_5C_7[p,q]): d(u) = 2, d(v) = 2\},$$
$$E_2(SC_5C_7[p,q]) = \{uv \in E(VC_5C_7[p,q]): d(u) = 2, d(v) = 3\},$$
$$E_3(SC_5C_7[p,q]) = \{uv \in E(VC_5C_7[p,q]): d(u) = 3, d(v) = 3\}$$

Using the definition of general Zagreb index and the edge partition (Table 4), we have from Table 1,

$$Z_{(a,b)}(SC_5C_7[p,q]) = \sum_{uv\in E(SC_5C_7[p,q])}(d(u)^a d(v)^b + d(u)^b d(v)^a)$$
$$= \sum_{uv\in E_1(SC_5C_7[p,q])}(d(u)^a d(v)^b + d(u)^b d(v)^a)$$

$$+\sum_{uv\in E_2(SC_5C_7[p,q])}(d(u)^a d(v)^b + d(u)^b d(v)^a)$$
$$+\sum_{uv\in E_3(SC_5C_7[p,q])}(d(u)^a d(v)^b + d(u)^b d(v)^a)$$
$$= |E_1(SC_5C_7[p,q])|\,(2^a2^b + 2^b2^a)$$
$$+|E_2(SC_5C_7[p,q])|\,(2^a3^b + 2^b3^a)$$
$$+|E_3(SC_5C_7[p,q])|\,(3^a3^b + 3^b3^a)$$
$$= 2p.2^{(a+b)} + 6p(2^a3^b + 2^b3^a) + (12pq - 9p).2.3^{(a+b)}$$
$$= p.2^{a+b+1} + 6p(2^a3^b + 2^b3^a) + 6p(4q-3).3^{(a+b)}.$$

Hence, the theorem. □

Corollary 3. From Theorem 3, we have the following results:

(i) $M_1(SC_5C_7[p,q]) = Z_{1,0}(SC_5C_7[p,q]) = 72pq - 20p,$

(ii) $M_2(SC_5C_7[p,q]) = \frac{1}{2}Z_{1,1}(SC_5C_7[p,q]) = 108pq - 41p,$

(iii) $F(SC_5C_7[p,q]) = Z_{2,0}(SC_5C_7[p,q]) = 216pq - 76p,$

(iv) $ReZM(SC_5C_7[p,q]) = Z_{(2,1)}(SC_5C_7[p,q]) = 648pq - 290p,$

(v) $SDD(SC_5C_7[p,q]) = Z_{(1,-1)}(SC_5C_7[p,q]) = 24pq - 3p,$

(vi) $R_\alpha(SC_5C_7[p,q]) = \frac{1}{2}Z_{(\alpha,\alpha)}(SC_5C_7[p,q]) = \left(4^\alpha + 6^\alpha - 3^{2(\alpha+1)}\right)p + 4.3^{2\alpha+1}.pq,$

(vii) $M^\alpha(SC_5C_7[p,q]) = Z_{(\alpha-1,0)}(SC_5C_7[p,q]) = 4(2^\alpha - 3^\alpha)p + 8.3^\alpha.pq.$

3. Conclusions

In this paper, we obtain the exact expressions of (a,b)-Zagreb index of some nanotubes covered by C_5 and C_7. Assigning some particular values to a, b, some well-established degree-based topological indices are derived. This work would help to understand the physicochemical properties, chemical reactivity, and biological activity of the nanostructures under consideration. The (a, b)-Zagreb index of several other structural features may be obtained for further analysis.

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Conflicts of Interest

The authors declare no conflict of interest.

References

1. Gutman, I.; Trinajestić, N. Graph theory and molecular orbitals total π-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **1972**, *17*, 535-538, https://doi.org/10.1016/0009-2614(72)85099-1.
2. Furtula, B.; Gutman, I.A. Forgotten Topological Index. *J. Math. Chem.* **2015**, *53*, 1184–90, https://doi.org/10.1007/s10910-015-0480-z.

3. Ranjini, P. S.; Lokesha,V.; Usha, A. Relation between phenylene and hexagonal squeeze using harmonic index. *Int.J.Graph Theory* **2013**, *1*, 116-121.
4. Li, X.; Zheng, J. A unified approach to the extremal trees for different indices. *MATCH Commun. Math. Comput.Chem.* **2005**, 54, 195-208.
5. Gutman, I.; Lepoviĉ, M. Choosing the exponent in the definition of the connectivity index. *J. Serb. Chem. Soc.* **2001**, *66*, 605-611, https://doi.org/10.2298/JSC0109605G.
6. Lokesha, V.; Deepika, T. Symmetric division deg index of tricyclic and tetra. cyclic graphs. *Int. J. Sci. Eng. Res.* **2016,** *7*, 53-55.
7. Alexander,V. Upper and lower bounds of symmetric division deg index. *Iran. J. Math. Chem.* **2014**, *52*, 91-98, https://dx.doi.org/10.22052/ijmc.2014.7357.
8. Gupta, C.K.; Lokesha, V.; Shwetha, B.S.; Ranjini, P.S. Graph operations on the symmetric division deg index of graphs. *Palestine. J. Math.* **2017**, *6*, 280-286.
9. Azari, M.; Iranmanesh, A. Generalized Zagreb index of graphs. *Studia Univ.Babes-Bolyai.* **2011**, *56*, 59-70.
10. Hayat, S.; Imran, M. Computation of Certain Topological Indices of Nanotubes Covered by C_5 and C_7. *Journal of Computational and Theoretical Nanoscience* **2015**, *12,* 1–9, https://doi.org/10.1166/jctn.2015.3761.
11. Mondal, S.; Bhosale A.; De N.; Pal A. Topological properties of some nanostructures. *Nanosystems: Physics, Chemistry, Mathematics* **2020**, *11*, 14–24, https://doi.org/10.17586/2220-8054-2020-11-1-14-24.
12. Farahani, M.R. The generalized Zagreb index of circumcoronene series of benzenoid. *J. Appl. Phys. Sci. Int.* **2015**, *3*, 99-105.
13. Muhammad, S.; Sardar, S.Z.; Farahani, M.R. The generalized zagreb index of capra-designed planar benzenoid series Cak(C6). *Open J. Math. Sci.* **2017**, *1*, 44–51.
14. Farahani, M.R., Kanna, M.R.R. Generalized Zagreb index of V-phenylenicnanotubes and nanotori. *J. Chem. Pharm. Res.* **2015**, *7*, 241-245.
15. De, N. Reduced second Zagreb index of product graphs. *Nanosystems: physics, chemistry, mathematics* **2020**, *11*, 131–137, https://doi.org/10.17586/2220-8054-2020-11-2-131-137.
16. Sridhara, G.; Kanna, M.R.R.; Indumathi, R.S. Computation of topological indices of graphene. *J. Nanomaterials*. **2015**, *2015*, https://doi.org/10.1155/2015/969348.
17. Shigehalli, V.S.; Kanabur, R. Computation of new degree based topological indices of graphene. *J. Math.* **2016,** *2016*, https://doi.org/10.1155/2016/4341919.
18. Mondal, S.; De, N.; Pal, A. Topological Indices of Some Chemical Structures Applied for the Treatment of COVID-19 Patients. *Polycyclic Aromatic Compounds* **2020**, https://doi.org/10.1080/10406638.2020.1770306.
19. Akhtar, S.; Imran, M.; Gao, W.; Farahani, M.R. On topological indices of honeycomb networks and grapheme networks. *Hacet. J. Math. Stat.* **2018**, *47*, 19-35, https://doi.org/10.15672/HJMS.2017.464.
20. Mondal, S.; De, N.; Pal, A. Topological properties of Graphene using some novel neighborhood degree-based topological indices. *International Journal of Mathematics for Industry* **2019**, *11*, https://doi.org/10.1142/S2661335219500060.
21. Baig, A.Q.; Imran, M.; Khalid, W.; Naeem, M. Molecular description of carbon graphite and crystal cubic carbon structure. *Canad. J. Chem.* **2017**, *95*, 674-686, https://doi.org/10.1139/cjc-2017-0083.
22. Gao, W.; Siddiqui, M.K.; Naeem, M.; Rahman, N.A. Topological characterization of carbon graphite and crystal cubic carbon structures. *Molecules.* **2017**, *22*, https://doi.org/10.3390/molecules22091496.
23. Raza, Z.; Sukaiti, M.E.K. M-Polynomial and Degree Based Topological Indices of Some Nanostructures. *Symmetry*. **2020**, 12, 831; https://doi.org/10.3390/sym12050831.
24. Zuo, X.; Liu, J.B.; Iqbal, H.; Ali, K.; Rizvi, S.T.R. Topological Indices of Certain Transformed Chemical Structures. *J. Chem*. **2020**, 2020, 3045646, https://doi.org/10.1155/2020/3045646.
25. Mufti, Z. S.; Amin, A.; Wajid, A.; Caudhary, S; Iqbal, H.; Ali, N. On Sanskruti and harmonic indices of a certain graph structure. *International Journal of Advanced and Applied Sciences* **2020**, 7, 1-8, https://doi.org/10.21833/ijaas.2020.02.001.

26. Babar, U.; Ali, H.; Arshad, S.H.; Sheikh, U. Multiplicative topological properties of graphs derived from honeycomb structure. *AIMS Mathematics* **2020,** 5, 1562-1587, https://doi.org/10.3934/math.2020107.
27. Prabhu, S.; Murugan, G.; Cary, M.; Arulperumjothi, M.; Liu, J.B. On certain distance and degree based topological indices of Zeolite LTA frameworks. *Mater. Res. Express* **2020**, 7, 055006, https://doi.org/10.1088/2053-1591/ab8b18.