Bond incident degree (BID) indices for some nanostructures

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The vertex degree of a molecular graph is the number of edges incident with that vertex. A great variety of topological indices are used in theoretical chemistry for predicting the physico-chemical properties of molecules, and many of them depend only on the vertex degrees of the corresponding molecular graph. Bond incident degree (BID) indices form a subclass of the class of all vertex degree based topological indices. In this paper, general formulae are reported for calculating BID indices of some nanostructures.

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1. Introduction

Denote the vertex set and edge set of a graph *G*, by *V(G)* and *E(G)* respectively. Let $|V(G)|=n(G)=n$ and $|E(G)|=m(G)=m$. Suppose that d_u is the degree of a vertex $u \in V(G)$ and uv is the edge connecting the vertices u and v [1]. In molecular graphs, the vertices correspond to atoms while the edges represent covalent bonds between atoms [2]. The number obtained from molecular graph, reflecting certain structural features of the molecule is called "molecular structure descriptor" or simply "topological index" [3]. A great variety of such indices are studied and used in theoretical chemistry [3-6]. Among them a large number of indices, depend only on vertex degrees of the molecular graph [4-6]. A considerable amount of these vertex-degree-based topological indices can be represented as the sum of edge contributions of graph [42-44]. These kind of vertex-degree-based topological indices are known as *bond incident degree indices* (BID indices in short) [42,43] whose general form [8-10,42-44] is:

$$TI(G) = \sum_{1 \le i < j \le \Delta} \theta_{i,j} x_{i,j} \qquad (1)$$

where $\theta_{i,j}$ is a non-negative real valued function depending on i , j *with* $\theta_{i,j} = \theta_{j,i}$, Δ is the maximum vertex degree in the graph G and $x_{i,j}$ is the number of edges in the graph *G* connecting the vertices of degrees *i* and *j*.

i): Let $\alpha \neq 0$ is a real number. If $\theta_{i,j} = (ij)^{\alpha}$, then TI is general Randić index [11] (variable second Zagreb index [41]). Moreover, if $\alpha = -\frac{1}{2}, 1, -1$ then TI is Randić index [12], second Zagreb index [13], modified second Zagreb index [14] respectively.

ii): If $\theta_{i,j} = (i+j)^{\beta}$, where $\beta \neq 0$ is a real number, then TI is the general sum-connectivity index [15]. If $= -\frac{1}{2}$, 1 , then TI is the sum-connectivity index [16], first Zagreb index [13] respectively.

iii): If $\theta_{i,j} = \left(\frac{i+j-2}{ij}\right)^{\gamma}$, where $\gamma \neq 0$ is a real number, then TI is the general atom-bond connectivity index [17]. For $\gamma = \frac{1}{2}, -3$, TI is the atom-bond connectivity index [18], augmented Zagreb index [19] respectively.

iv): If $\theta_{i,j} = \left(\frac{2\sqrt{ij}}{i+j}\right)^{\lambda}$, where $\lambda > 0$ is a real number, then TI is the ordinary generalized geometric–arithmetic index [20]. For $\lambda = 1$, TI is the first geometric-arithmetic index [21].

v): If $\theta_{i,j} = \frac{2}{i+j}$, then TI is the harmonic index [22].

vi): If $\theta_{i,j} = |i-j|$, then TI is the Albertson index [23].

vii): If $\theta_{i,j} = \frac{lni}{i} + \frac{lnj}{j}$, then TI is logarithm of the first multiplicative Zagreb index [31].

viii): If $\theta_{i,j} = ln(i+j)$, then TI is logarithm of the second multiplicative Zagreb index [31].

ix): If $\theta_{i,j} = ln\, i + lnj$, then TI is logarithm of the modified first multiplicative Zagreb index [32].

Nanotechnology is a technology that deals with small structures or small sized materials. A nanometer (nm) is one billionth of a meter, or $10^{-9}m$. Nanostructured materials are those with at least one dimension falling in nanometer scale, and include nanoparticles (including quantum dots, when exhibiting quantum effects), nano-rods and nanowires, thin films, and bulk materials made of nanoscale building blocks or consisted of nanoscale structures. Many technologies have been explored to fabricate nanostructures [24].

M.V. Diudea [25, 26] was the first chemist who considered the problem of computing topological indices of nanostructures. A.R. Ashrafi and his co-authors [27, 28]

continued this pioneering work of M.V. Diudea. In recent years, the problem of computing topological indices of nanostructures has attracted substantial attention from many researchers [33-40].

In this paper, closed form formulae for calculating the BID indices of several nanostructures are given. These formulae generalize some already reported results.

2. Main results and discussion

The Nano-cones are constructed from a graphene sheet by removing a wedge and joining the edges produces a cone with a single regular polygon defects at the apex. Let us denote by $NC_k[n]$ an arbitrary Nano-cone, where k is the number of edges in the single regular polygon and n is the number of hexagonal layers surrounding the regular polygon (see Fig.1 for $NC_5[4]$ Nano-cone).

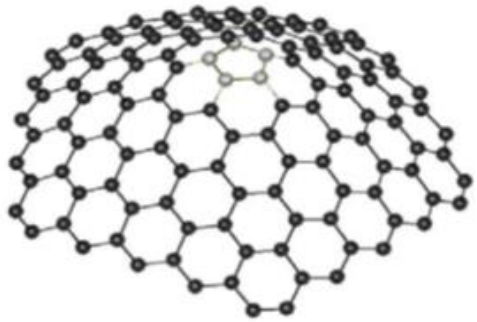

Fig. 1. A $NC_5[4]$ Nano-cone [A. R. Ashrafi, H. Shabani, Optoelectron. Adv. Mater.-Rapid Commun., 4 (2010), 1874 - 1876.]

It can be easily seen that $C_k[n]$ has $\frac{k}{2}(n+1)(3n+2)$ edges and contains only vertices of degree 2 and 3. Moreover, the number of edges in the last layer is $k(2n+1)$ from which k edges are of the type (2,2) and remaining are of the type (2,3), hence:

$$x_{2,2}(C_k[n]) = k,\ x_{2,3}(C_k[n]) = k(2n+1) - k = 2nk,$$

$$x_{3,3}(C_k[n]) = \frac{k}{2}(n+1)(3n+2) - k(2n+1)$$

Then from Equation (1), it follows that

$$TI(C_k[n]) = \theta_{2,2}k + \theta_{2,3}2nk + \frac{kn}{2}(3n+1)\theta_{3,3}\,.$$

This formula can be considered as a generalization of some results already reported in [33-35].

If we substitute

$$\theta_{i,j} = \left(\frac{i+j-2}{ij}\right)^{-3}$$

in Equation (1), then TI is the augmented Zagreb index (AZI) and hence

$$AZI(C_k[n]) = 8k + 16nk + \frac{729kn}{128}(3n+1)$$

Now, let us compute BID indices for a special type of k-polyomino system. A k-polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular 4k-cycle of side length one. In other words, it is an edge-connected union of cells [29]. Let us take $k = 2$ and denote by Z_n the 2-polyomino zigzag chain (see the Fig. 2).

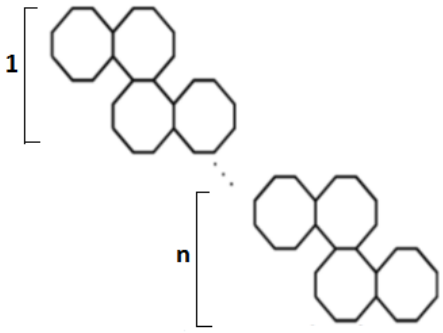

Fig. 2. The zig-zag chain of 8-cycles Z_n

For the Z_n graph, the non-zero values of $x_{i,j}$ are given below:

$$x_{2,2}(Z_n) = 12n+4,\ x_{2,3}(Z_n) = 8n,\ x_{3,3}(Z_n) = 8n-3.$$

Using these values Equation (1), we get

$$TI(Z_n) = \theta_{2,2}(12n+4) + 8n\theta_{2,3} + \theta_{3,3}(8n-3) \qquad (2)$$

and by simple calculations, one have

$$AZI(C_k[n]) = \frac{2009}{8}n - \frac{139}{64}.$$

In [36], first geometric-arithmetic index was calculated for Z_n graph, which can also be calculated from Equation (2).

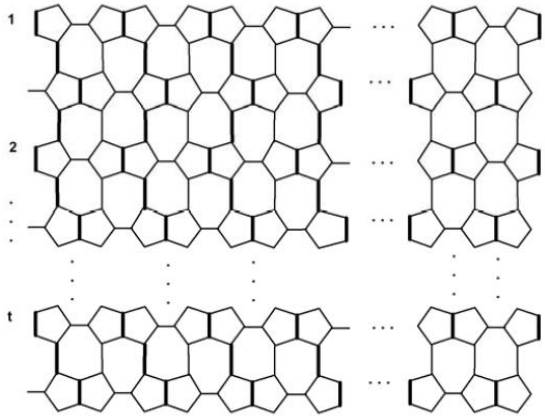

Fig. 3. A 2-Dimensional Lattice of HC5C7[r,t] [A. R. Ashrafi, M. Ghojavand, Digest Journal of Nanomaterials and Biostructures, 3 (2008), 209 - 214]

Now, we compute BID indices for some nanotubes. In 1991 Lijima [30] discovered carbon nanotubes as multi-walled structures. These nanotubes form an interesting class of carbon nano-materials which can be imagined as rolled sheets of graphite about different axes. Furthermore, carbon nanotubes show remarkable mechanical properties. Experimental studies have shown that they belong to the stiffest and elastic known materials. One of the main distinctive characteristics of carbon nanotubes is the use of mathematical tools for modeling of their physic-chemical properties.

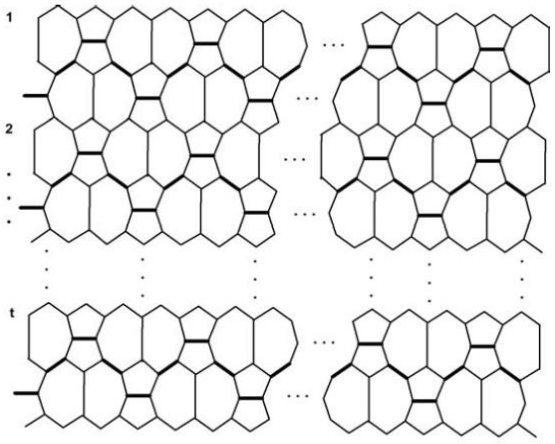

Fig. 4. A 2-Dimensional Lattice of $SC_5C_7[r,t]$ [A. R. Ashrafi, M. Ghojavand, Digest Journal of Nanomaterials and Biostructures, 3 (2008), 209 - 214.]

Firstly, let us consider the $H_1 = HC_5C_7[r,t]$ and $H_2 = SC_5C_7[r,t]$ nanotubes. A C_5C_7 net is a trivalent decoration made by alternating C_5 and C_7 cycles. This net can cover either a torus or a cylinder. See the Fig. 3 and Fig. 4 for 2-dimensional lattices of H_1 and H_2 respectively, where r is the number of heptagons in the first row and t is shown in the aforementioned figures. The non-zero values of $x_{i,j}$ for these two nanotubes are given below [37]:

$$x_{2,3}(H_1) = 4r,\ x_{3,3}(H_1) = 6rt - r - 4r = 6rt - 5r$$

$$x_{2,2}(H_2) = t,\ x_{2,3}(H_2) = 6t,\ x_{3,3}(H_2) = 6rt - r - 7t$$

Hence, after substituting these values in Equation (1) we arrive at,

$$TI(H_1) = 4r\theta_{2,3} + \theta_{3,3}(6rt - 5r) \quad (3)$$

$$TI(H_2) = t\theta_{2,2} + 6t\theta_{2,3} + \theta_{3,3}(6rt - r - 7t) \quad (4)$$

In [37], first geometric-arithmetic index was calculated for $HC_5C_7[r,t]$ and $SC_5C_7[r,t]$. Using Equations (3) and (4), one can easily calculate any BID index for $HC_5C_7[r,t]$ and $SC_5C_7[r,t]$ nanotubes.

Now, we consider the $H_3 = HAC_5C_7[r,t]$, $H_4 = HAC_5C_6C_7[r,t]$ and $H_5 = VAC_5C_7[r,t]$ nanotubes. For the figures of these nanotubes see [7, 38]. The values of non-zero $x_{i,j}$ for these two nanotubes are given below [7, 38]:

$$x_{1,3}(H_3) = r,\ x_{2,3}(H_3) = 2r,\ x_{3,3}(H_3) = 12rt - 3r$$

$$x_{1,3}(H_4) = 2r,\ x_{2,3}(H_4) = 4r,\ x_{3,3}(H_4) = 24rt - 6r$$

$$x_{2,2}(H_5) = 2r,\ x_{2,3}(H_5) = 8r,\ x_{3,3}(H_5) = 12rt - 4r$$

From Equation (1), it follows that

$$TI(H_3) = r\theta_{1,3} + 2r\theta_{2,3} + \theta_{3,3}(12rt - 3r) \quad (5)$$

$$TI(H_4) = 2r\theta_{1,3} + 4r\theta_{2,3} + \theta_{3,3}(24rt - 6r) \quad (6)$$

$$TI(H_5) = 2r\theta_{2,2} + 8r\theta_{2,3} + \theta_{3,3}(12rt - 4r) \quad (7)$$

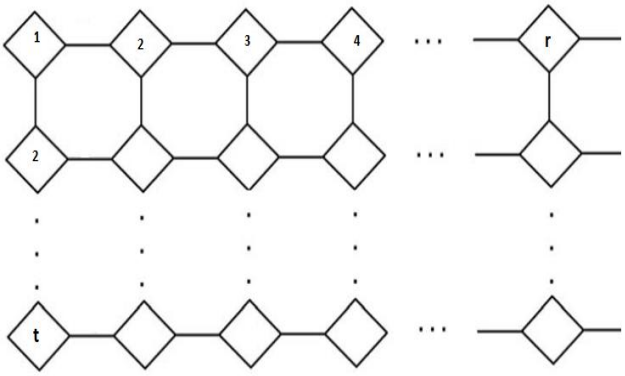

Fig. 5. A 2-Dimensional Lattice of $TUC_4C_8(R)[r,t]$

In [38], first geometric-arithmetic index was calculated for $HAC_5C_7[r,t]$ and $HAC_5C_6C_7[r,t]$ nanotubes. In [7], Randić and sum-connectivity indices were calculated for $VAC_5C_7[r,t]$ nanotube. Using Equations (5), (6) and (7), we can calculate any BID index for these three nanotubes.

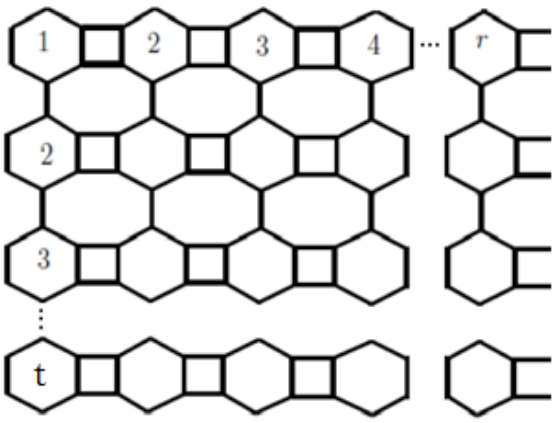

Fig. 6. A 2-Dimensional Lattice of $TUC_4C_8(S)[r,t]$

Finally, let us consider the nanotubes $H_6 = TUC_4C_8(R)[r,t]$ $H_7 = TUC_4C_8(S)[r,t]$ and $H_8 = TUC_4C_6C_8\ [r,\ t]$. See the Fig. 5, Fig. 6 and Fig. 7 for 2-dimensional lattices of H_6, H_7 and H_8 respectively. From these figures, it can be easily seen that the non-zero values of $x_{i,j}$ for the H_6, H_7 and H_8 nanotubes are:

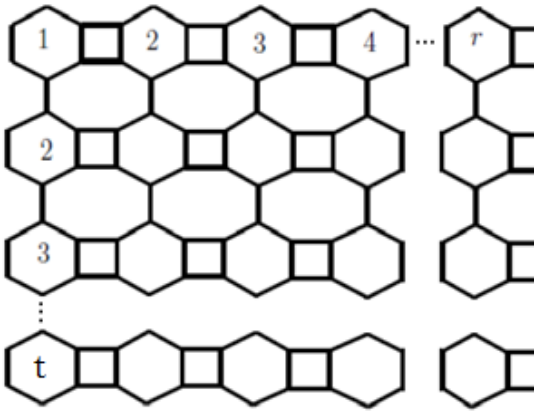

Fig. 7. A 2-Dimensional Lattice of $TUC_4C_6C_8\ [r,\ t]$

$$x_{2,3}(H_6) = 4r,\ x_{3,3}(H_6) = 6rt - 5r$$

$$x_{2,2}(H_7) = 2r, x_{2,3}(H_7) = 4r,\ x_{3,3}(H_7) = 12rt - 8r$$

$$x_{2,3}(H_8) = 4r,\ x_{3,3}(H_8) = 2rt + 9r$$

Hence, after substituting these values in Equation (1) we arrive at,

$$TI(H_6) = 4r\theta_{2,3} + \theta_{3,3}(6rt - 5r) \quad (8)$$

$$TI(H_7) = 2r\theta_{2,2} + 4r\theta_{2,3} + \theta_{3,3}(12rt - 8r) \quad (9)$$

$$TI(H_8) = 4r\theta_{2,3} + \theta_{3,3}(2rt + 9r) \quad (10)$$

In [39], first geometric-arithmetic index was calculated for $TUC_4C_8(R)[r,t]$ and $TUC_4C_8(S)[r,t]$ nanotubes. In [40], first geometric-arithmetic and atom-bond connectivity indices were calculated for $TUC_4C_6C_8\ [r,\ t]$ nanotube. Using Equations (8), (9) and (10), we can calculate any BID index for these three nanotubes.

At the end, we summarize all the results in the following table:

Graph	**Value of *TI***
$NC_k[n]$	$k\theta_{2,2} + 2nk\theta_{2,3} + \frac{kn}{2}(3n+1)\theta_{3,3}$
Z_n	$\theta_{2,2}(12n+4) + 8n\theta_{2,3} + \theta_{3,3}(8n-3)$
$HC_5C_7[r,t]$	$4r\theta_{2,3} + \theta_{3,3}(6rt - 5r)$
$SC_5C_7[r,t]$	$t\theta_{2,2} + 6t\theta_{2,3} + \theta_{3,3}(6rt - r - 7t)$
$HAC_5C_7[r,t]$	$r\theta_{1,3} + 2r\theta_{2,3} + \theta_{3,3}(12rt - 3r)$
$HAC_5C_6C_7[r,t]$	$2r\theta_{1,3} + 4r\theta_{2,3} + \theta_{3,3}(24rt - 6r)$
$VAC_5C_7[r,t]$	$2r\theta_{2,2} + 8r\theta_{2,3} + \theta_{3,3}(12rt - 4r)$
$TUC_4C_8(R)[r,t]$	$4r\theta_{2,3} + \theta_{3,3}(6rt - 5r)$
$TUC_4C_8(S)[r,t]$	$2r\theta_{2,2} + 4r\theta_{2,3} + \theta_{3,3}(12rt - 8r)$
$TUC_4C_6C_8\ [r,\ t]$	$4r\theta_{2,3} + \theta_{3,3}(2rt + 9r)$

References

[1] F. Harary, Graph Theory, Addison-Wesley, Reading, MA, (1969).

[2] W. Karcher, J. Devillers, Environmental Chemistry and Toxicology, Springer, (1990).

[3] J. Devillers, A.T. Balaban (Eds.), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon and Breach, Amsterdam, (1999).

[4] I. Gutman, B. Furtula (Eds.), Novel Molecular Structure Descriptors—Theory and Applications vols. I-II, Univ. Kragujevac, Kragujevac, (2010).

[5] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, (2000).

[6] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley-VCH, Weinheim, (2009).

[7] M. R. Farahani, Advances in Materials and Corrosion. **2,** 33 (2013).

[8] J. Rada, R. Cruz, I. Gutman, Chemical Physics Letters. **572**, 154 (2013).

[9] H. Deng, J. Yang, F. Xia, Computers and Mathematics with Applications **61**, 3017 (2011).

[10] I. Gutman, Croat. Chem. Acta **86**, 351 (2013).

[11] X. Li, I. Gutman, Mathematical Aspects of Randić- type Molecular Structure Descriptors, Univ. Kragujevac, Kragujevac, Serbia, (2006).

[12] M. Randić, J. Am. Chem. Soc. **97**, 6609 (1975).

[13] I. Gutman, N. Trinajstić, Chem. Phys. Lett. **17**, 535 (1972).

[14] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, Croat.Chem. Acta. **76,** 113 (2003).
[15] B. Zhou, N. Trinajstić, J. Math. Chem. **47**, 210 (2010).
[16] B. Zhou, N. Trinajstić, J. Math. Chem. **46**, 1252 (2009).
[17] R. Xing, B. Zhou, Filomat **26**, 683 (2012).
[18] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, Indian J. Chem. **37A**, 849 (1998).
[19] B. Furtula, A. Graovac, D. Vukičević, J. Math. Chem. **48**, 370 (2010).
[20] Mehdi Eliasi, Ali Iranmanesh, Applied Mathematics Letters **24**, 582 (2011).
[21] D. Vukičević, B. Furtula, J. Math. Chem. **46**, 1369 (2009).
[22] S. Fajtlowicz, Congr. Numer. **60**, 187 (1987).
[23] M. Albertson, Ars Comb. **46**, 219 (1997).
[24] G. Cao, Y. Wang, World Scientific Series in Nanoscience and Nanotechnology, **2**, (2011).
[25] M. V. Diudea, M. Stefu, B. Parv, P. E. John, Croat. Chem. Acta, **77**, 111 (2004).
[26] P. E. John, M. V. Diudea, Croat. Chem. Acta **77**, 127 (2004).
[27] A. R. Ashrafi, F. Rezaei, MATCH Commun. Math. Comput. Chem. **57**, 243 (2007).
[28] A. R. Ashrafi, A. Loghman, Ars Comb. **80**, 193 (2006)
[29] D. A. Klarner, Polyominoes, In: J. E. Goodman, J. O'Rourke, (eds.) Handbook of Discrete and Computational Geometry, Chapter 12, pp. 225–242, CRC Press, Boca Raton (1997).
[30] S. Lijima, Nature **354**, 56 (1991).
[31] I. Gutman, Bull. Int. Math. Virt. Inst. **1**, 13 (2011).
[32] M. Eliasi, I. Gutman, A. Iranmanesh, MATCH Commun. Math. Comput. Chem. **68**, 217 (2012).
[33] L. Yang, H. Hua, Optoelectron. Adv. Mat. **6**, 660 (2012).
[34] A. R. Ashrafi, H. Shabani, Optoelectron. Adv. Mat. **4**, 1874 (2010).
[35] A. Khaksar, M. Ghorbani, H. R. Maimani, Optoelectron. Adv. Mat. **4**, 1868 (2010).
[36] M. Ghorbani, M. Ghazi, Digest Journal of Nanomaterials and Biostructures **5**, 837 (2010).
[37] A. Iranmanesh, M. Zeraatkar, Optoelectron. Adv. Mat. **4**, 1852 (2010).
[38] A. Iranmanesh, M. Zeraatkar, Optoelectron. Adv. Mat. **5**, 790 (2011).
[39] S. Chen, W. Liu, J. Comput. Theor. Nanosci. **7**, 1993 (2010).
[40] M. Ghorbani, H. Mesgarani, S. Shakeraneh, Optoelectron. Adv. Mat. **5**, 324 (2011).
[41] S. Nikolić, A. Miličević, Croat. Chem. Acta **77**, 97 (2004).
[42] D. Vukičević, M. Găsperov, Croat. Chem. Acta **83** (3), 243 (2010).
[43] D. Vukičević, J. Durdević, Chem. Phys. Lett. **515**, 186 (2011).
[44] B. Hollas, MATCH Commun. Math. Comput. Chem. **54**, 177 (2005).

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