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New Definition of Atomic Bond Connectivity Index to Overcome the Deficiency of Structure Sensitivity and Abruptness in the Existing Definition

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Abstract

Topological Index (TI) is a numerical value associated with the molecular graph of the compound. Smoothness property states that a TI is good if its Structure Sensitivity (SS) is as large as possible and its Abruptness (Abr) is small. In 2013, Gutman proved that Atomic Bond Connectivity (ABC) index has small SS and high Abr. In this paper, we defined reverse Atomic Bond Connectivity (ABC) index to overcome this problem. Moreover, we computed reverse ABC index for Silicon Carbides, Bismith Tri-Iodide and Dendrimers.

Keywords: Atomic Bond Connectivity (ABC) index, Bismith Tri-Iodide, Dendrimers, reverse ABC index, Silicon Carbides, structure sensitivity, topological index

Introduction

Topological Indices (TIs) enable us to collect information about algebraic structures and give us a mathematical approach to understand the properties of algebraic structures [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. Many criteria were put forward to check the quality of a TI. The first criterion was proposed by Randic. Afterwards, many such criteria were proposed. A famous one is that it should change gradually with gradual change in structure. This property is known as the smoothness property [12] of TIs and it has two measures namely Structure Sensitivity (SS) and Abruptness (Abr).

Let G be a molecular graph and TI is its topological index, then G = Γ(G) which is a set having all connected sets of G obtained by the replacement of edges with each other. Then

$$SS(TI,G) = \frac{1}{\Gamma(G)} \sum_{\gamma\in\Gamma(G)} \left| \frac{TI(G)-TI(\gamma)}{TI(G)} \right| \quad (1)$$

$$Abr(IT,G) = \max_{\gamma\in\Gamma(G)} \left| \frac{TI(G)-TI(\gamma)}{TI(G)} \right|. \quad (2)$$

As per Equation (1), SS is the average relative sensitivity of TI to minor changes in the structure of the graph G. As per Equation (2), Abr indicates how a small basic change may cause a big change in TI.

Among degree based TIs, the Augmented Zagreb Index (AZI) has the most noteworthy structure affectability followed by the Second Zagreb Index (M2). For example, for trees having 10 vertices, SS(AZI) = 0.118 and SS(M2) = 0.103, trailed by SS(M1) = 0.073 and so forth, while for trees with 12 vertices, SS(M2) = 0.089, SS(AZI) = 0.086, trailed by SS(M1) = 0.058 and so on. A similar result holds for other inspected estimations of n. Subsequently, at any rate for trees the degree based TIs with the best structure affectability are AZI and M2 and these seem by all accounts to be better than the different indices considered. Along these lines, for n = 12 M2 and AZI have the most extreme unexpectedness (Abr (M2) = 0.270 and Abr (AZI) = 0.0217, trailed by Abr (M1) = 0.149). The ABC index has the structure affectability, which can't help contradicting the cases that ABC is a generally excellent proportion of spreading subordinate thermodynamic properties of alkanes.

Estrada [13] introduced the ABC index. It is defined as $ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u(G)+d_u(2)-2}{d_u(G).d_v(G)}}$.

Recently, Gutman [12] proved that ABC index is not good because it has small SS and high Abr. To overcome this problem, we defined the reverse ABC index as follows,

$$CABC(G) = \sum_{uv\in CE(G)} \sqrt{\frac{C_u(G)+C_u(2)-2}{C_u(G).C_v(G)}}$$

where $c_v = \Delta(G) - d_g(v) + 1$ and Δ(G) is the maximum degree of vertex [14].

Moreover, we computed the reverse ABC index and calculated it for Silicon Carbides, Bismith Tri-Iodide and Dendrimers. Figures (1-4) [15] represent the molecular graph of Silicon Carbide $Si_2\ C_3\ -[p,q]$. Figures (5-8) [16] represent the molecular graph of Silicon Carbide $Si_2\ C_3-\text{II}[p,q]$. Figures (9-12) [17] represent the molecular graph of Silicon Carbide Si2C3 −III[p,q]. Figures (13-16) [17] represent the molecular graph of Silicon Carbide $Si_2\ C_3-III\ [p,q]$.

Figures (17-19) [18] show the molecular graph of Bismuth Tri-Iodide chin and sheet.

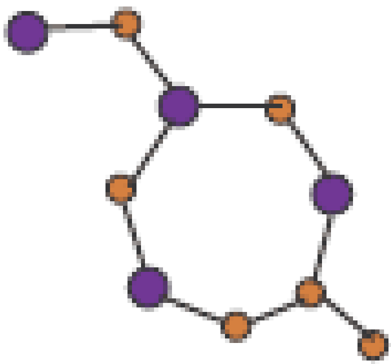

Figure 1. $Si_2\ C_3 - I[1,1]$

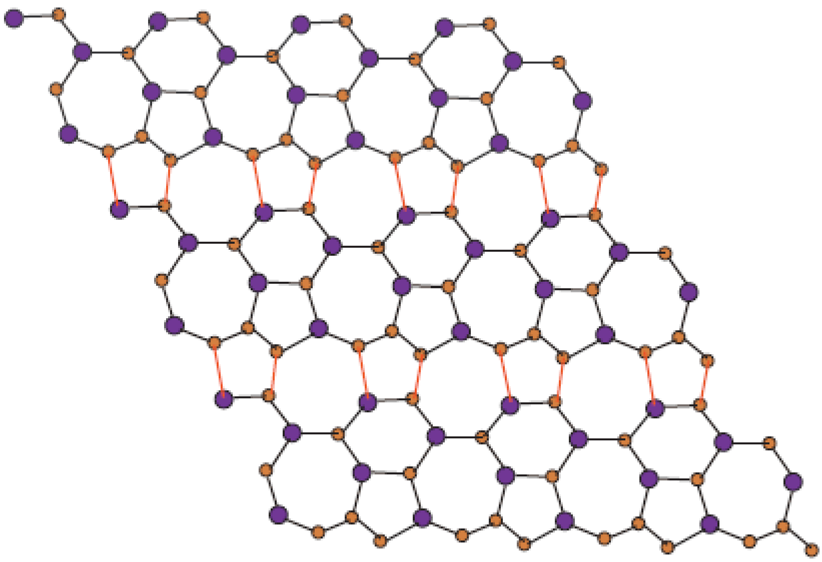

Figure 2. $Si_2\ C_3 - I[4,3]$

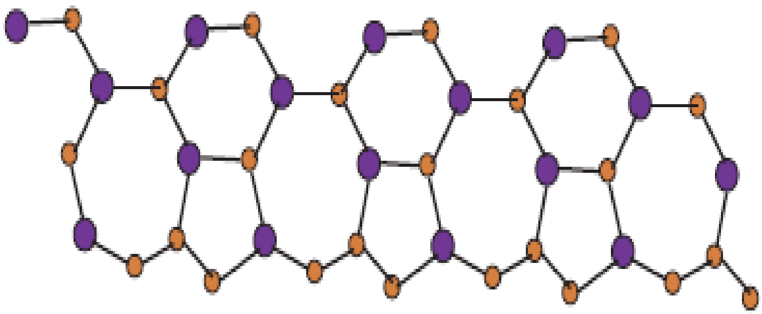

Figure 3. $Si_2\ C_3 - I[4,1]$

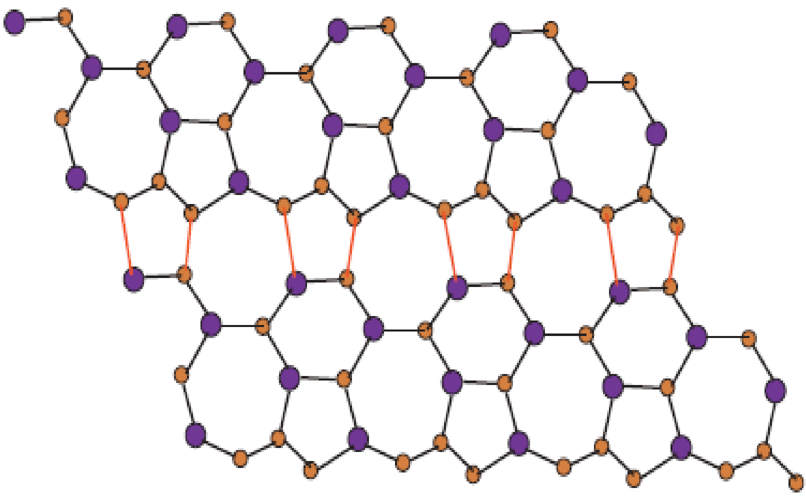

Figure 4. $Si_2\ C_3 - I[4,2]$

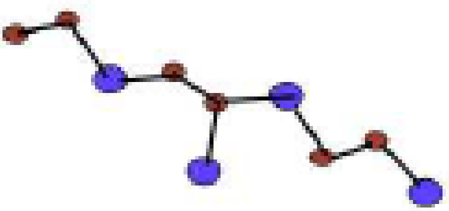

Figure 5. $i_2\ C_3 - II[1,1]$

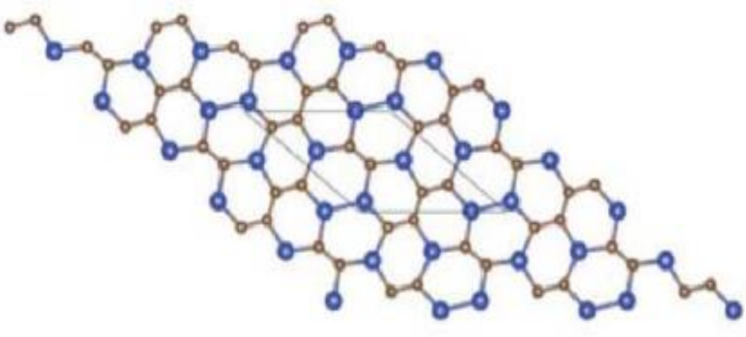

Figure 6. $Si_2\ C_3 - II[3,3]$

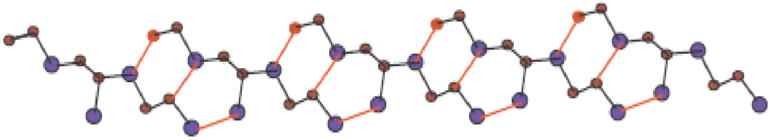

Figure 7. $Si_2\ C_3 - II[5,1]$

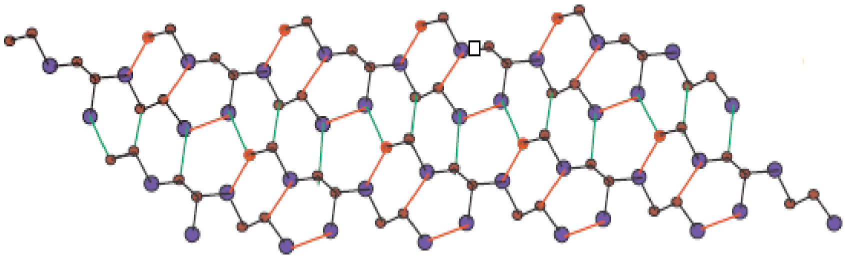

Figure 8. $Si_2\ C_3 - II[5,2]$

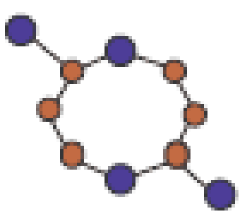

Figure 9. $Si_2\ C_3 - III[1,1]$

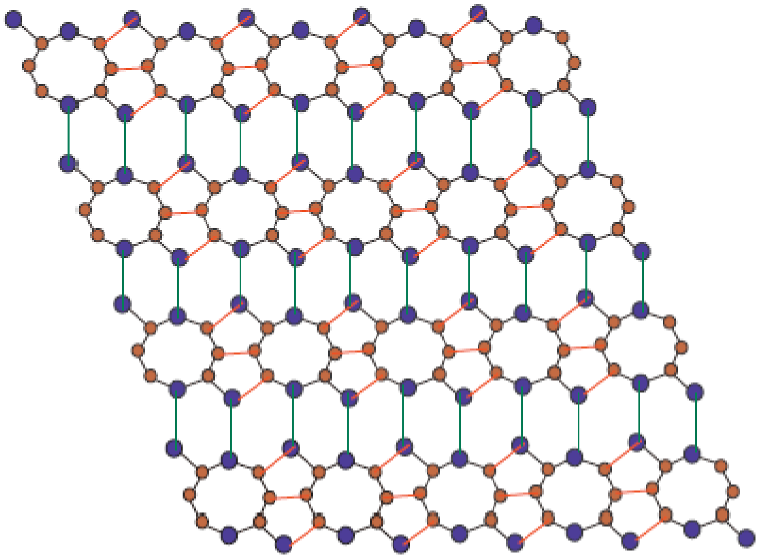

Figure 10. $Si_2\, C_3 - III[5,4]$

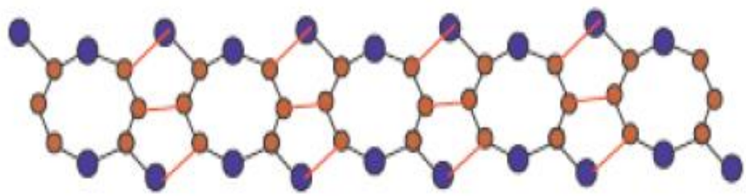

Figure 11. $Si_2\, C_3 - III[5,1]$

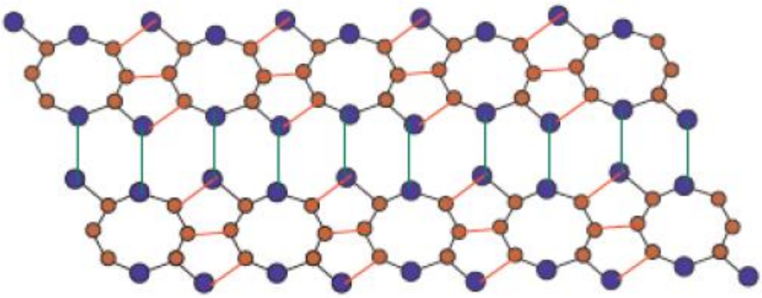

Figure 12. $Si_2\, C_3 - III[5,2]$

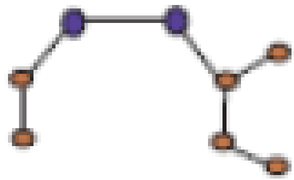

Figure 13. $Si\ C_3 - III[1,1]$

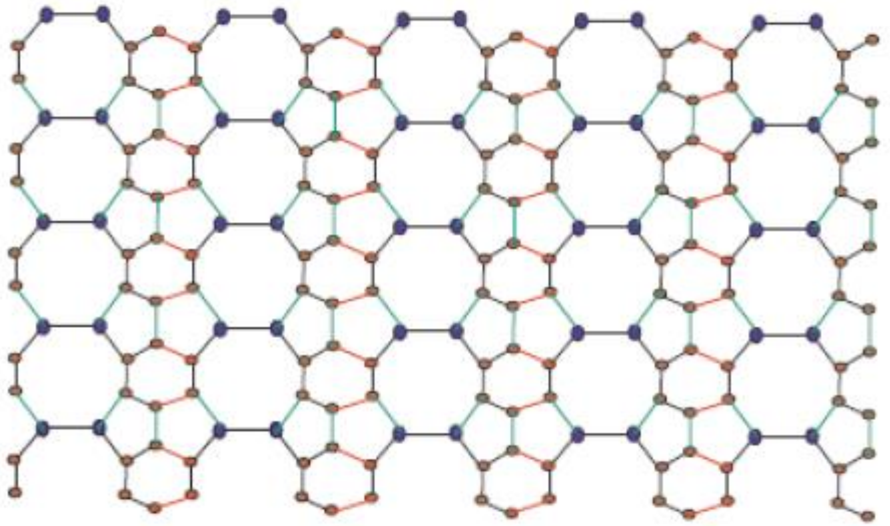

Figure 14. $Si\ C_3 - III[5,5]$

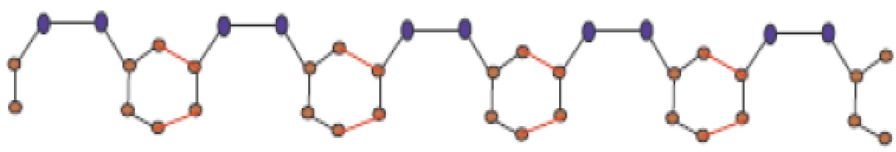

Figure 15. $Si\ C_3 - III[5,1]$

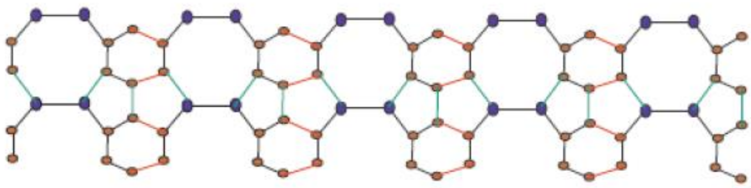

Figure 16. $Si\ C_3 - III[5,2]$

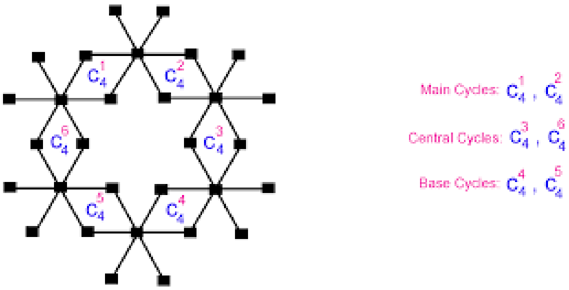

Figure 17. Unit Cell (Bismuth Tri-Iodide)

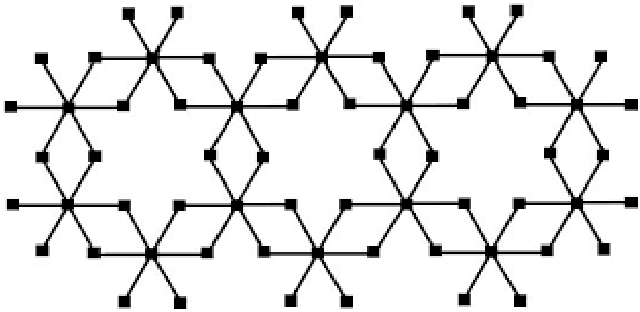

Figure 18. The Chain for m = 3 (Bismuth Tri-Iodide)

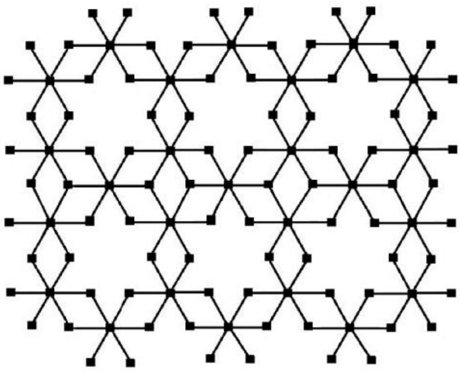

Figure 19. Sheet for m = 2 and n = 3 (Bismuth Tri-Iodide)

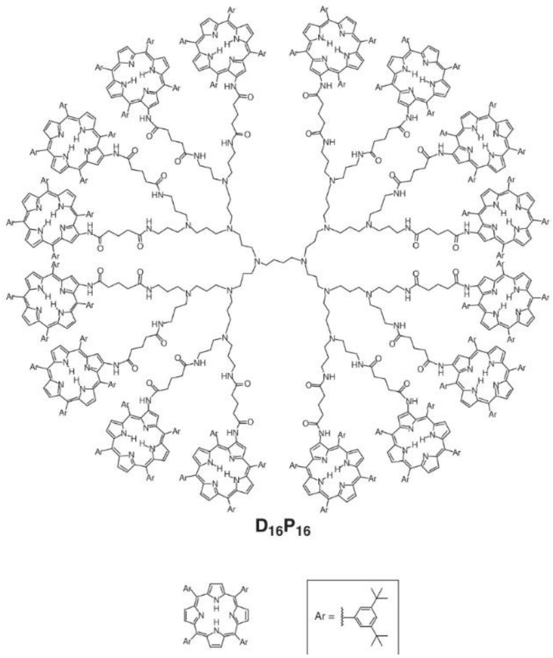

Figure 20. Prophyrin Dendrimer D_nP_n

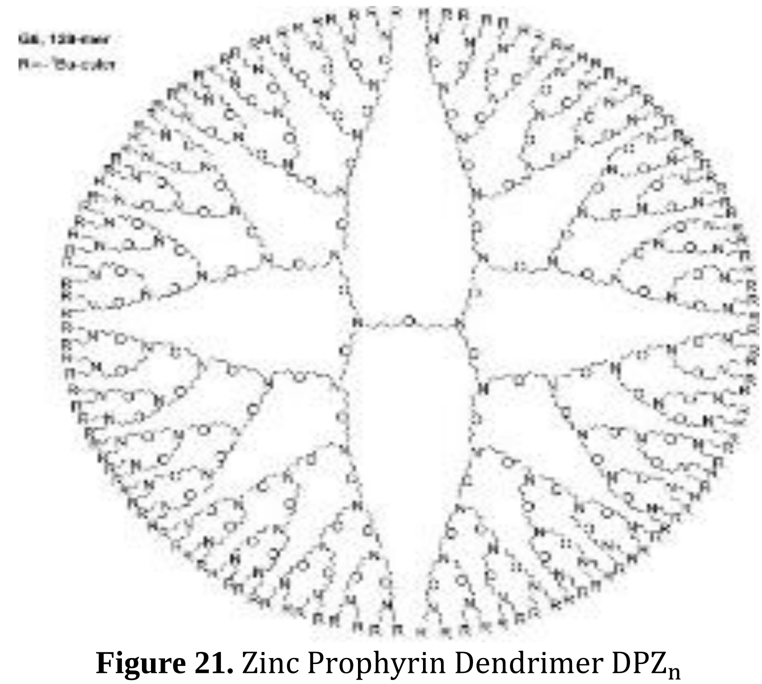

Figure 21. Zinc Prophyrin Dendrimer DPZ_n

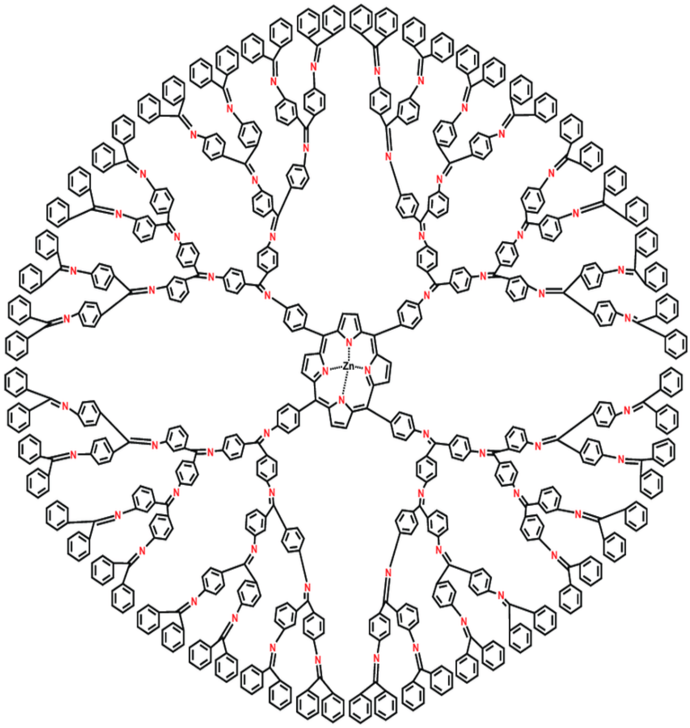

Figure 22. Zinc Porphyrin Dendrimer DPZ_n

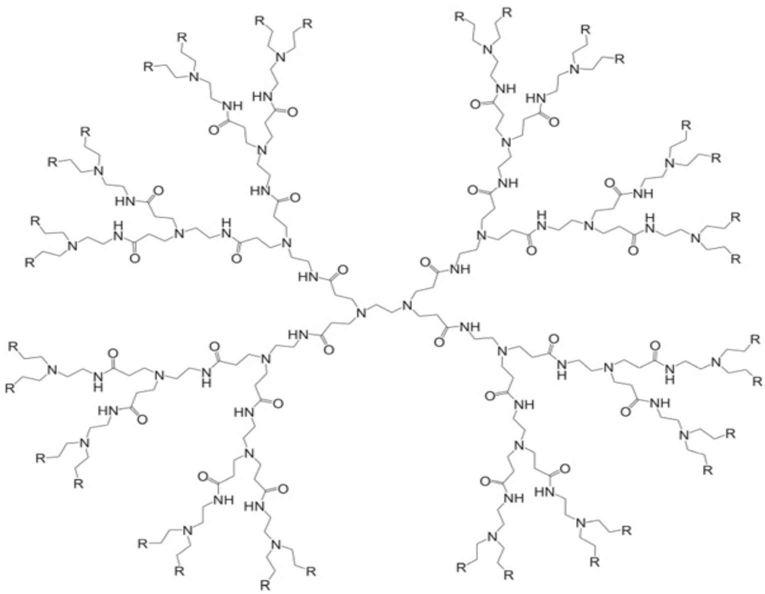

Figure 23. Poly (Ethylene Amide Amine) Dendrimer PETAA

Table 1. Reverse E(Si_2C_3–I[p,q])

(C_u, C_v)	Frequency
(3,2)	1
(3,1)	1
(2,2)	p+2q
(2,1)	2(3p+4q)-9
(1,1)	3p(5q-3)-13q+7

Table 2. Reverse E(Si_2C_3–$II[p,q]$

(C_u, C_v)	Frequency
(3,2)	2
(3,1)	1
(2,2)	2(p+q)
(2,1)	2(4p+4q-7)
(1,1)	15pq-13(p+q)+11

2. Main Result

Theorem 2.1 Reverse ABC indices for Silicon Carbides are

(1) $CABC(Si_2C_3 - I[p,q]) = \frac{1}{\sqrt{2}} 7p + 5\sqrt{2}q + \frac{1}{3}(\sqrt{6} - 12\sqrt{2}),$

(2) $CABC(Si_2C_3 - II[p,q]) = 5\sqrt{2}p + 5\sqrt{2}q + \frac{1}{3}(\sqrt{6} - 18\sqrt{2}),$

(3) $CABC(Si_2C_3 - III[p,q]) = 4\sqrt{2}p + 5\sqrt{2}q - \frac{1}{3}(13\sqrt{5}),$

(4) $CABC(Si_2C_3 - III[p,q]) = \frac{1}{\sqrt{2}} 9p + 3q + \frac{1}{\sqrt{6}}(2\sqrt{6} - 7\sqrt{3} + 2).$

Proof. 1 From the reverse E(Si_2C_3–I[p,q]), we have

$$CABC(Si_2C_3 - I[p,q]) = \sum_{uv \in CESi_2C_3 - II[p,q]} \sqrt{\frac{c_u + c_u - 2}{c_u . c_v}}$$

$$= \sqrt{\frac{3+2-2}{3 \times 2}}(1) + \sqrt{\frac{3+1-2}{3 \times 1}}(1) + \sqrt{\frac{2+2-2}{2 \times 2}}(p + 2q)$$

$$+ \sqrt{\frac{2+1-2}{2 \times 1}}(6p + 8q - 9) + \sqrt{\frac{1+1-2}{1 \times 1}}(15pq - 9p - 13q + 7)$$

$$= \frac{1}{\sqrt{2}} 7p + 5\sqrt{2}q + \frac{1}{3}(\sqrt{6} - 12\sqrt{2}).$$

2. From the reverse E (Si_2C_3–II [p,q]), we have

$$CABC(Si_2C_3 - II[p,q]) = \sum_{uv\in CESi_2C_3-II[p,q]} \sqrt{\frac{c_u + c_u - 2}{c_{u}.c_v}}$$

$$= \sqrt{\frac{3+2-2}{3\times 2}}(2) + \sqrt{\frac{3+1-2}{3\times 1}}(1) + \sqrt{\frac{2+2-2}{2\times 2}}(2p+2q)$$

$$+ \sqrt{\frac{2+1-2}{2\times 1}}(8p+8q-14) + \sqrt{\frac{1+1-2}{1\times 1}}(15pq - 13p - 13q + 11)$$

$$= 5\sqrt{2}p + 5\sqrt{2}q + \frac{1}{3}(\sqrt{6} - 18\sqrt{2}).$$

Table 3. Degree E ($Si_2C_3 - III$[p,q])

(C_u, C_v)	**Frequency**
(3,1)	2
(2,2)	2(q+1)
(2,1)	4(2p+2q-3)
(1,1)	5p(3q-2p)-13q+8

Table 4. Reverse E ($SiC_3 - III$[p,q])

(C_u, C_v)	**Frequency**
(3,2)	2
(3,1)	1
(2,2)	3(p-1)+2q
(2,1)	2(3p+2q-4)
(1,1)	(12p-8) (q-1)

3. From the reverse E ($Si_2C_3 - III$[p,q]), we have

$$CABC(Si_2C_3 - III[p,q]) = \sum_{uv\in CE(Si_2C_3-II[p,q])} \sqrt{\frac{c_u + c_v - 2}{c_{u}.c_v}}$$

$$= \sqrt{\frac{3+1-2}{3\times 1}}(2) + \sqrt{\frac{2+2-2}{2\times 2}}(2q+2) + \sqrt{\frac{2+1-2}{2\times 1}}(8p+8q$$
$$-12) + \sqrt{\frac{1+1-2}{1\times 1}}(15pq-10p-13q+8)$$
$$= 4\sqrt{2}p + 5\sqrt{2}q - \frac{1}{3}(13\sqrt{5}).$$

4. From the reverse E ($SiC_3 - III$ [p,q]), we have

$$CABC(Si_2C_3 - III[p,q]) = \sum_{uv\in CE(SiC_3(-III[p,q])} \sqrt{\frac{c_u + c_v - 2}{c_{u.}c_v}}$$
$$= \sqrt{\frac{3+2-2}{3\times 2}}(2) + \sqrt{\frac{3+1-2}{3\times 1}}(1) +$$
$$\sqrt{\frac{2+2-2}{2\times 2}}(3p+2q-3) + \sqrt{\frac{2+1-2}{2\times 1}}(6p+4q-8) +$$
$$\sqrt{\frac{1+1-2}{1\times 1}}(12pq-12p-8q+8)$$
$$= \frac{1}{\sqrt{2}}9p + 3q + \frac{1}{\sqrt{6}}(2\sqrt{6} - 7\sqrt{3} + 2).$$

Theorem 2.2 Reverse ABC indices for Bismith Tri-Iodide chain and sheet are

(1) $C\ ABC(m - Bil_3[m,n]) = \frac{1}{\sqrt{30}}[(20+40\sqrt{6})m + (40+8\sqrt{6})]$

(2)$C\ ABC\ (Bil_3(m\times n)) = \frac{1}{2\sqrt{5}}(48+6\sqrt{15})mn + \frac{1}{\sqrt{30}}(20 + 16\sqrt{6})m + (20+16\sqrt{6} - 9\sqrt{10})n + \frac{1}{\sqrt{30}}$(20-8$\sqrt{6}$

Proof. 1 From the reverse E($m - Bil_3[m,n]$), we have

$$CABC(m - Bil_3[m,n]) = \sum_{uv\in CE(m-Bil_3[m,n])} \sqrt{\frac{c_u + c_v - 2}{c_{u.}c_v}}$$
$$= \sqrt{\frac{6+1-2}{6\times 1}}(4m+8) + \sqrt{\frac{5+1-2}{5\times 1}}(20m+4)$$

$$= \frac{1}{\sqrt{30}}[(20+40\sqrt{6})m + (40+8\sqrt{6})].$$

2. From the reverse E $(Bil_3(m \times n))$, we have

$$CABC\left(Bil_3(m \times n)\right) = \sum_{uv \in CE(Bil_3(m \times n))} \sqrt{\frac{c_u + c_v - 2}{c_{u}.c_v}}$$

$$= \sqrt{\frac{6+1-2}{6\times1}}(4m + 4n + 4) + \sqrt{\frac{5+1-2}{5\times1}}(12mn + 8m + 8n - 4)$$
$$+ \sqrt{\frac{4+1-2}{4\times1}}(6mn - 6n)$$

$$= \frac{1}{2\sqrt{5}}\left(48 + 6\sqrt{15}\right)mn + \frac{1}{\sqrt{30}}(20+16\sqrt{6})m + (20 + 16\sqrt{6} - 9\sqrt{10})n + \frac{1}{\sqrt{30}}(20-8\sqrt{6}).$$

Table 5. Reverse E($m - Bil_3[m,n]$)

$(C_{u,}C_{v,})$	**Frequency**
(6,1)	4m+8
(5,1)	20m+4

Table 6. Reverse E($Bil_3(m \times n)$)

$(C_{u,}C_{v,})$	**Frequency**
(6,1)	4m+4n+4
(5,1)	12mn+8m+8n-4
(4,1)	6mn-6n

Theorem 2.3 Reverse ABC indices for Dendrimers are

(1) $C\,ABC\,(D_n p_n) = \frac{1}{3}\,(186\sqrt{3} + 84\sqrt{2} + 26)n - \frac{1}{3}(9\sqrt{2} + 10)$

(2) $C\,ABC\,(PETIM) = \frac{1}{\sqrt{2}}(2^{n+4} + 2^{n+1} + 6.2^{n}) - \frac{1}{\sqrt{2}}24$

(3) $C\,ABC\,(DPZ_n) = \frac{1}{3}(60\sqrt{3} + 12\sqrt{2} + 32).2^n + \frac{1}{3}\,(4\text{-}24\sqrt{3})$

(4) $C\,ABC(PETAA) = (2\sqrt{3}+8\sqrt{2} + 24)\,2^n - (\sqrt{3}+4\sqrt{2} + 9)$

Table 7. Reverse E ($D_n\, P_n$)

(C_u, C_v)	**Frequency**
(4,2)	2n
(4,1)	124n
(3,3)	5(2n-1)
(3,2)	48n-6
(2,2)	13n
(2,1)	8n

Table 8. Reverse E (*PETIM)*

(C_u, C_v)	Frequency
(3,2)	2^{n+1}
(2,2)	$2^{n+4} - 18$
(2,1)	$6(2^{n}$ -1)

Proof. 1. From the reverse E ($D_n\, P_n$), we have

$$CABC(D_n\, P_n) = \sum_{uv \in CE(D_n\, P_n)} \sqrt{\frac{c_u + c_v - 2}{c_u . c_v}}$$

$$= \sqrt{\frac{4+2-2}{2\times 2}}(2n) + \sqrt{\frac{4+1-2}{4\times 1}}(124n) + \sqrt{\frac{3+3-2}{3\times 3}}\,(10n-5) + \sqrt{\frac{3+2-2}{3\times 2}}(48n-6) + \sqrt{\frac{2+2-2}{2\times 1}}(13n) + \sqrt{\frac{2+1-2}{2\times 1}}\,(8n)$$

$$= \frac{1}{3}(186\sqrt{3} + 84\sqrt{2} + 26)n - \frac{1}{3}(9\sqrt{2} + 10).$$

2. From the reverse E(*PETIM*), we have

$$CABC(D_n\, P_n = \sum_{uv \in CE(D_n\, P_n)} \sqrt{\frac{c_u + c_v - 2}{c_u . c_v}}$$

$$= \sqrt{\frac{3+2-2}{3\times 2}}(2^{n+1}) + \sqrt{\frac{2+2-2}{2\times 2}}(2^{n+4}-18) + \sqrt{\frac{2+1-2}{2\times 1}}\,(6.2^{n}-6)$$

$$= \frac{1}{\sqrt{2}}(2^{n+4} + 2^{n+1} + 6.2^{n}) - \frac{1}{\sqrt{2}}\,24.$$

Table 9. Reverse E (DPZ_n)

($C_{u,}C_{v,}$)	**Frequency**
(3,3)	$16.2^{n}-4$
(4,1)	$40.2^{n}-16$
(3,3)	$8.2^{n}-16$
(2,1)	4

Table 10. Reverse E (PETAA)

($C_{u,}C_{v,}$)	**Frequency**
(3,2)	4.2^{n}
(3,1)	$4.2^{n}-2$
(2,2)	$16.2^{n}-8$
(2,1)	$20.2^{n}-9$

3. From the reverse E (DPZ_n), we have

$$C\,ABC(D_n P_n) = \sum_{uv\in CE(D_n P_n)} \sqrt{\frac{c_u + c_v - 2}{c_{u}.c_{v}}}$$

$$= \sqrt{\frac{3+3-2}{3\times 3}}(16.2^{n}-4) + \sqrt{\frac{4+1-2}{4\times 1}}(40.2^{n}-16)$$

$$= \sqrt{\frac{3+2-2}{3\times 2}}(8.2^{n}-16) + \sqrt{\frac{2+2-2}{2\times 1}}(4)$$

$$= \frac{1}{3}(60\sqrt{3} + 12\sqrt{2} + 32).2^{n} + \frac{1}{3}(4\text{-}24\sqrt{3}).$$

4. From the reverse E (*PETAA)*, we have

$$C\ ABC(PETAA) = \sum_{uv\in CE(PETAA)} \sqrt{\frac{c_{u} + c_{v} - 2}{c_{u}.c_{v}}}$$

$$= \sqrt{\frac{4+2-2}{2\times 2}}(4.2^{n}) + \sqrt{\frac{4+1-2}{4\times 1}}(4.2^{n}-2)$$

$$+ \sqrt{\frac{3+2-2}{3\times 2}}(16.2^{n}-8) + \sqrt{\frac{2+1-2}{2\times 1}}(20.2^{n}-9)$$

$$= (2\sqrt{3} + 8\sqrt{2} + 24)\ 2^{n} - \left(\sqrt{3} + 4\sqrt{2} + 9\right).$$

4. Conclusion

TIs have found application in different regions of science, material science, arithmetic, informatics, biology, and so on and their most basic use to date is in Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Activity Relationships (QSAR). From the perspective of usefulness, TI for which the absolute value of r is below 0.8 can be depicted as useless. ABC index has small SS and high Abr [1]. In this paper, we defined the reverse ABC index to overcome this problem.

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