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Reciprocal Atom-bond connectivity and Fourth Atom-bond connectivity indices for Polyphenylene structure of molecules

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Polyphenylene is a class of polycyclic aromatic compounds that has varied applications in biochemistry and biology. A numerical measure that defines the characteristics of a chemical structure is called topological index. In chemical graph theory, Estrada et al. proposed the degree-based topological indices known as Atom-bond connectivity index (ABC) [4]. A new version of ABC index is Fourth Atom-bond connectivity index (ABC_4) proposed by M. Ghorbani et al. [6]. A valuable predictive index in the study of the heat of formation of alkanes, the strain energy of cycloalkanes is ABC index. Based on this, numerous articles were reported. In this study, novel indices, Reciprocal Atom-bond Connectivity ($RABC$) and Reciprocal Fourth Atom-bond connectivity($RABC_4$) indices were proposed and a comparative study of correlation with properties of octane isomers were given. It was observed that these indices showed good correlation for physico chemical properties of octane isomers. Subsequently, Reciprocal Atom-bond connectivity and Reciprocal Fourth Atom-bond connectivity indices for Polyphenylene structure of molecules were computed.

KEYWORDS

Polyphenylene structure of molecules; ABC index; ABC_4 index.

Introduction

The chemical graph theory is a branch of mathematics, which applies graphs as tools for representing chemical structures/compounds. As graph theory has varied applications in every field in which every example is considered as a graph and hence further study is possible. For instance, it is applied in communication networks, transport networks and other fields by considering the network as a graph [2, 23, to name a few]. Similarly, in chemistry, a chemical structure is considered as a graph from which a treasure of information can be studied. Topological indices are one such tool which gives information about the physical and chemical properties of the compound considered under the study [7, 9, 11, 14, 19]. A detailed analysis of a chemical compound could be drawn based on the values of topological indices. This study is called quantitative structure activity relationship (QSAR) based on which a lot of research is being conducted worldwide [1, 16, 20, 18, 24]. To be very precise, in representing a chemical compound as a graph, the molecules are considered as nodes/vertices and the covalent bonds between them are represented as edges. This results in a graphical structure on which the study takes place. In mathematical chemistry, the double bonds of a compound

when represented as a graph, are considered as a single edge. This is done as all the research in mathematical chemistry considers only simple graphs. Also, the hydrogen atoms of a compound are nullified when it is converted to a graph [13, 15, 17, 22, 26].

A real number related to a graph is a topological index. Many topological indices have been introduced and have found significant applications in the fields of pharmaceutical, chemical and drugs manufacturing. The study of aromatic hydrocarbons has attracted a lot of researchers in which the TIs provide a lot of information about the aromatic compounds (Hydro Carbons) [3, 5, 8, 12]. Let $G = (V, E)$ be a graph consists of a non-empty set of vertices V and a set of edges E respectively [10, 21].

Definition 1.1 *Estrada et al., [4] introduced Atom-bond Connectivity index and it is stated as,*

$$ABC(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{d_G(v)+d_G(\omega)-2}{d_G(v)d_G(\omega)}}$$

Definition 1.2 *M. Ghorbani et al., [6] introduced fourth Atom-bond connectivity index $ABC_4(G)$ is defined as*

$$ABC_4(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{S_G(v)+S_G(\omega)-2}{S_G(v)S_G(\omega)}}$$

The main objective of this work was proposing novel indices like $RABC$ and $RABC_4$ and making a comparative study of the existing indices with these novel indices of Polyphenylene structure of molecules. Motivated by the works of Estrada et al., and M. Ghorbani et al., an attempt was made to define novel indices as given below.

Definition 1.3 *The novel indices introduced in this work are RABC and $RABC_4$ and they are defined as*

$$RABC(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{d_G(v)d_G(\omega)}{d_G(v)+d_G(\omega)-2}}$$

$$RABC_4(G) = \sum_{v\omega \in E(G)} \sqrt{\frac{S_G(v)S_G(\omega)}{S_G(v)+S_G(\omega)-2}}$$

where $S_G(v)$ represents the sum of the degrees of all vertices adjacent to the vertex v, i.e. $S_v = \sum_{\omega \in N_G(v)} d\omega$.

*On Chemical applicability of the **RABC** and **$RABC_4$** indices*

The results of $RABC$ and $RABC_4$ are authenticated using the data set of octane isomers(*http://www.moleculardescripters.eu/dataset.htm*). The dataset includes the properties (Boiling-point, melting-point, critical temperature, critical pressure, mean radius, molar refraction, entropy, enthalpy of vaporization, standard enthalpy of vaporization, density, acentric factor, surface tension and heat of formation). The correlation of $RABC$ and $RABC_4$ with all these properties were studied. Surprisingly, it was found that $RABC$ and $RABC_4$ satisfy the properties standard enthalpy of vaporization ($HVAP$) and entropy(S) of octane isomers with correlation coefficient $r \geq 0.935$ and $r \geq -0.855$. The structure property relationship models of $RABC$ and $RABC_4$ have been developed as below and represented as shown in Figure 1.

Tables 1 and 2 show correlation coefficient between existing indices ABC , ABC_4 and novel indices $RABC$, $RABC_4$ for physicochemical properties of octane isomers.

$$HVAP = (111.691)ABC(G) - 8.065$$

$$\& \; HVAP = (21.641)RABC(G) + 5.073.$$

$$S = (7.821)ABC_4(G) + 22.7275$$

$$\& \; S = (212.045)RABC_4(G) - 9.291.$$

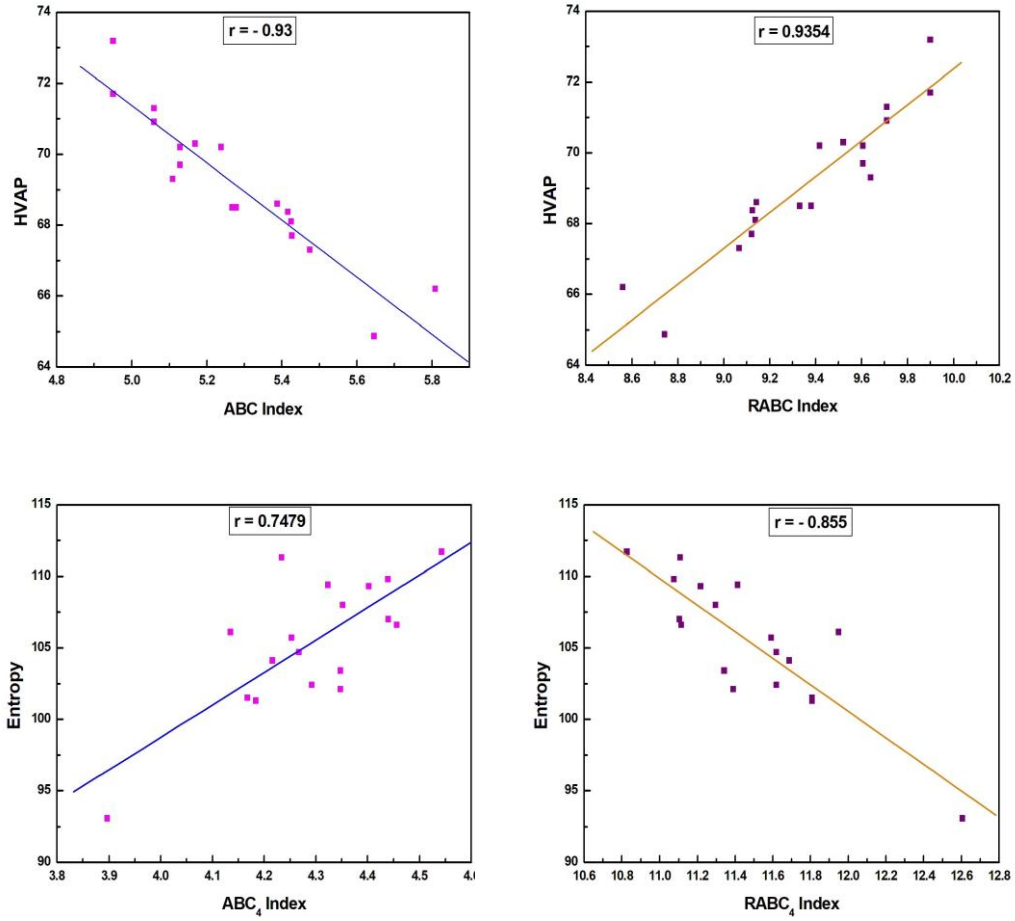

FIGURE 1 Correlation of ABC , $RABC$, ABC_4 and $RABC_4$ indices with $HVAP$ and entropy of octane isomers

TABLE 1 The correlation Coefficients between ABC and $RABC$ indices

Index	***HVAP***	***BP***	***CP***	***D***	$-H_f$	***ST***
ABC	**-0.93**	−0.862	−0.624	−0.023	0.8933	−0.713
$RABC$	**0.935**	0.878	0.638	0.032	−0.902	0.7334

TABLE 2 The correlation Coefficients between ABC_4 and $RABC_4$ indices

Index	***S***	***AF***	***HVAP***	***DHAVP***	***BP***	***CP***	***D***	R_m^2	$-H_f$	***MV***	***ST***
ABC_4	**0.748**	0.7435	0.577	0.6697	0.4784	−0.099	−0.6915	0.5598	−0.4845	0.6856	0.1142
$RABC_4$	**-0.855**	−0.8273	−0.653	−0.742	−0.528	0.171	0.7223	−0.65	0.532	−0.719	−0.1192

Polyphenylene structure

The structure of polyphenylene considered in this study is represented in Figure 2. It is observed that it is a cycle of 6 hexagons connected with an edge in between every hexagon which is nothing but the bond between two carbon atoms.

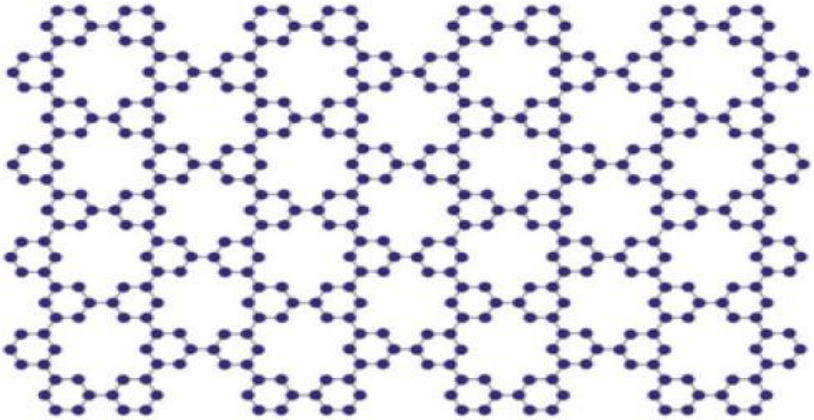

FIGURE 2 Polyphenylene Structure of Molecules $[m, n]$

These cycles of 6 hexagons relate to other cycles of 6 hexagons with carbon-carbon bonds. In other words, it is a polymer of benzenoid aromatic compounds. A lot of research has been done on this since few years as it has arisen many applications like single group of polymers, which could be changed to another one. For example, an electrical insulator can be transformed in electrical conductor by using doping with electron acceptor or donor. Polyphenylenes attract a lot of attention because of its special feature of thermal and thermo-oxidative stabilities.

Recently Xuewu Zuo, et al. [25] studied some degree-based numerical invariants (sum of degrees of incident vertices) of Polyphenylene structure of molecules through M–Polynomials.

In this study, novel indices including $RABC$ and $RABC_4$ were proposed and validated for properties of octane isomers. The same novel indices were computed for Polyphenylene structure for degree-based indices (sum of degrees of incident vertices and sum of degrees of neighboring vertices).

From Figure 2, Polyphenylene structure with m rows and n columns has the cardinality of vertex set to be $24mn + 12m$ and that of edge set to be $30mn + 13m - n$. Tables 3 and 4 show the edge partition of $P[m, n]$ with respect to degree sum of incident vertices and neighboring degree sum of adjacent vertices respectively.

TABLE 3 The edge partition of $P[m, n]$

$[d_G(v), d_G(\omega)]$ where $v\omega \in E(G)$	*No. of Edges*
$E_1(2,2)$	$4m + 8n$
$E_2(2,3)$	$24mn - 4m + 4n$
$E_3(3,3)$	$6mn - m + n$

TABLE 4 The edge partition of $P[m, n]$

$[S_G(v), S_G(\omega)]$ where $v\omega \in E(G)$	*No. of Edges*
$E_1(4,5)$	$4m + 8n$
$E_2(5,7)$	$4m + 8n$
$E_3(6,7)$	$24mn - 8m - 4n$
$E_4(7,7)$	$6mn - m + n$

Main results

***ABC** and **RABC** indices of Polyphenylene Structure of Molecules **P**[**m**, **n**]*

Theorem 4.1 *The ABC index of $P[m,n]$ is given by*

$$\left(\frac{2097}{100}\right)mn-\left(\frac{667}{1000}\right)m+\left(\frac{9151}{1000}\right)n$$

Proof.

$$ABC(G)=\sum_{v\omega\in E(G)}\sqrt{\frac{d_G(v)+d_G(\omega)-2}{d_G(v)d_G(\omega)}}$$

$$=\sum_{v\omega\in E_1(G)}\sqrt{\frac{2+2-2}{(2)(2)}}+\sum_{v\omega\in E_2(G)}\sqrt{\frac{2+3-2}{(2)(3)}}+\sum_{v\omega\in E_3(G)}\sqrt{\frac{3+3-2}{(3)(3)}}$$

$$=(4m+8n)\left(\frac{707}{1000}\right)+(24mn-4m+4n)\left(\frac{707}{1000}\right)+(6mn-m+n)\left(\frac{667}{1000}\right)$$

$$=\left(\frac{2097}{100}\right)mn-\left(\frac{667}{1000}\right)m+\left(\frac{9151}{1000}\right)n$$

Theorem 4.2 *The RABC index of $P[m,n]$ is given by*

$$\left(\frac{2147}{50}\right)mn-\left(\frac{3}{2}\right)m+\left(\frac{1847}{100}\right)n$$

Proof.

$$RABC(G)=\sum_{v\omega\in E(G)}\sqrt{\frac{d_G(v)d_G(\omega)}{d_G(v)+d_G(\omega)-2}}$$

$$=\sum_{v\omega\in E_1(G)}\sqrt{\frac{(2)(2)}{2+2-2}}+\sum_{v\omega\in E_2(G)}\sqrt{\frac{(2)(3)}{2+3-2}}+\sum_{v\omega\in E_3(G)}\sqrt{\frac{(3)(3)}{3+3-2}}$$

$$=(4m+8n)\left(\frac{707}{500}\right)+(24mn-4m+4n)\left(\frac{707}{500}\right)+(6mn-m+n)\left(\frac{3}{2}\right)$$

$$=\left(\frac{2147}{50}\right)mn-\left(\frac{3}{2}\right)m+\left(\frac{1847}{100}\right)n$$

TABLE 5 depicts ABC and $RABC$ of $P[m,n]$ for varied values of $[m,n]$

$[m,n]$	[1,1]	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]
$ABC(G)$	29.454	100.848	214.182	369.456	566.67	805.824	1086.918
$RABC(G)$	59.91	205.7	437.37	754.92	1158.35	1647.66	2222.85

Table 5: The ABC and $RABC$ indices of $P[m,n]$.

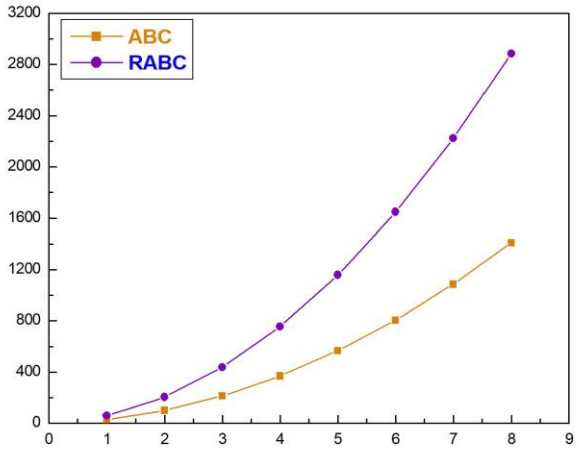

FIGURE 3 Graphical comparison between ABC and $RABC$ on $[m,n]$

ABC_4 and $RABC_4$ indices of Polyphenylene $P[m,n]$

Theorem 4.3 *The ABC_4 index of $P[m,n]$ is given by*

$$\left(\frac{61}{4}\right)mn-\left(\frac{417}{5000}\right)m+\left(\frac{373}{50}\right)n$$

Proof.

$$ABC_4(G)=\sum_{v\omega\in E(G)}\sqrt{\frac{S_G(v)+S_G(\omega)-2}{S_G(v)S_G(\omega)}}$$

$$=\sum_{v\omega\in E_1(G)}\sqrt{\frac{4+5-2}{(4)(5)}}+\sum_{v\omega\in E_2(G)}\sqrt{\frac{5+7-2}{(5)(7)}}+\sum_{v\omega\in E_3(G)}\sqrt{\frac{6+7-2}{(6)(7)}}+\sum_{v\omega\in E_4(G)}\sqrt{\frac{7+7-2}{(7)(7)}}$$

$$=(4m+8n)\left(\frac{74}{125}\right)+(4m+8n)\left(\frac{107}{200}\right)+(24mn-8m-4n)\left(\frac{64}{125}\right)+(6mn-m+n)\left(\frac{99}{200}\right)$$

$$=\left(\frac{61}{4}\right)mn-\left(\frac{417}{5000}\right)m+\left(\frac{373}{50}\right)n$$

Theorem 4.4 *The $RABC_4$ index of $P[m,n]$ is given by*

$$\left(\frac{1473}{25}\right)mn-\left(\frac{169}{50}\right)m+\left(\frac{227}{10}\right)n$$

Proof.

$$RABC_4(G)=\sum_{v\omega\in E(G)}\sqrt{\frac{S_G(v)S_G(\omega)}{S_G(v)+S_G(\omega)-2}}$$

$$=\sum_{v\omega\in E_1(G)}\sqrt{\frac{(4)(5)}{4+5-2}}+\sum_{v\omega\in E_2(G)}\sqrt{\frac{(5)(7)}{5+7-2}}+\sum_{v\omega\in E_3(G)}\sqrt{\frac{(6)(7)}{6+7-2}}+\sum_{v\omega\in E_4(G)}\sqrt{\frac{(7)(7)}{7+7-2}}$$

$$=(4m+8n)\left(\frac{169}{100}\right)+(4m+8n)\left(\frac{187}{100}\right)+(24mn-8m-4n)\left(\frac{39}{20}\right)+(6mn-m+n)\left(\frac{101}{50}\right)$$

$$=\left(\frac{1473}{25}\right)mn-\left(\frac{169}{50}\right)m+\left(\frac{227}{10}\right)n$$

TABLE 6 depicts ABC_4 and $RABC_4$ of $P[m,n]$ for varied values of $[m,n]$

$[m,n]$	[1,1]	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]
$ABC_4(G)$	22.627	75.573	159.38	273.506	418.133	593.26	798.886
$RABC_4(G)$	78.24	274.32	588.24	1020	1569.6	2237.04	3022.32

Table 6: The ABC_4 and $RABC_4$ indices of $P[m,n]$.

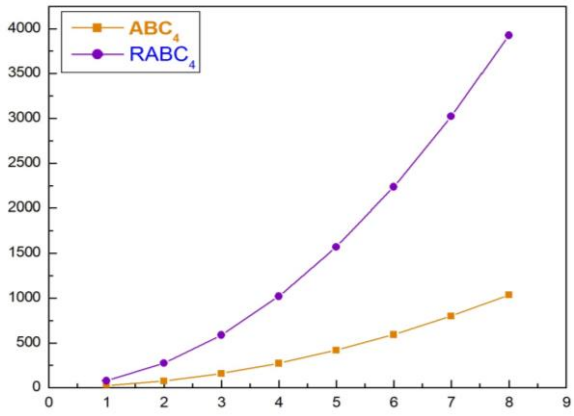

FIGURE 4 Graphical comparison between ABC_4 and $RABC_4$ on $P[m,n]$

Comparison of indices

The defined topological indices were calculated for different pairs of values of $m = n$. It was noticed that the values of topological indices increased as $m = n$ increased. This was shown numerically and graphically using Tables 5 and 6 and Figures 3 and 4.

Conclusion

In this study, novel indices namely $RABC$ and $RABC_4$ were proposed and a comparative study of correlation with properties of octane isomers was given. It was observed that these indices show good correlation for physico chemical properties of octane isomers. The correlation coefficients between ABC and $RABC$ indices were correlated well for the property $HVAP$ while ABC_4 and $RABC_4$ indices were positively correlated with the property S. Later, $RABC$ and $RABC_4$ for Polyphenylene structure of molecules were computed. For this, it was observed that the topological indices increased with the increase in the $m = n$.

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