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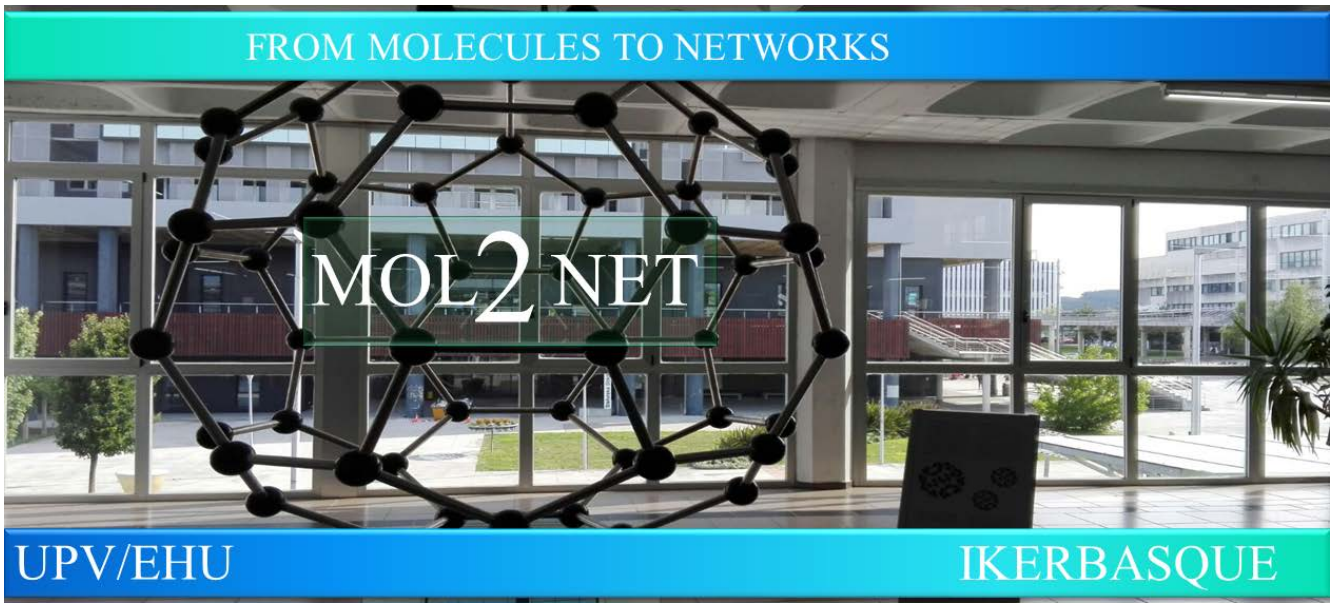

Significance of the fourth atom bond connectivity index in predicting the physicochemical properties of polycyclic aromatic hydrocarbons

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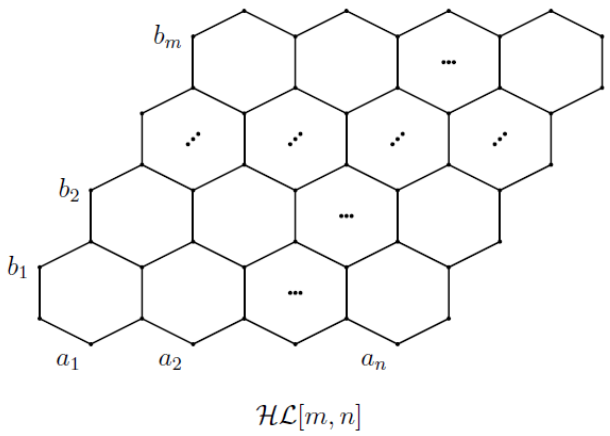
Graphical Abstract	**Abstract.**
	Chemical graph theory mainly deals with quantitative structure-activity (QSAR) and structure-property relationships (QSPR) studies. A large number of topological indices have been introduced by various eminent researchers. These



$\mathcal{HL}[m,n]$

are found to be useful in those studies. In this paper, we focused on the fourth atom bond connectivity index and how it can be used for the accurate prediction of physicochemical properties of polycyclic aromatic hydrocarbons, considered as graphene fragments. These properties were boiling point, molar entropy, acentric factor, logarithm of octanol-water partition coefficient, and Kovats retention index.

Introduction

Graph theory is used to mathematically model molecules to gain insight into the physical properties of chemical compounds. A graph is a pair $G \cong (V,E)$ where V is a set whose elements are called vertices and E is a set whose elements are called edges. In chemical graph theory, atoms correspond to vertices and bonds to edges. Hydrogen atoms are not usually taken into account in a chemical graph. A chemical graph is finite connected and non directed. It can be considered as simple or as multigraph or pseudograph. The degree of a vertex $v \in G$ is the number of edges incident to v and it is denoted by $d_G(v)$. It is common to use, in addition, alternative definitions of degree to characterize the chemical element that represents the vertex or its chemical environment. A topological index (TI) is a mapping that assigns a real number to a chemical graph that is correlated to various physicochemical properties of a chemical compound and it is invariant under graph isomorphisms. Biological activities, as well as physicochemical and chemical properties of organic compounds, are correlated with their molecular structure. The quantitative relationship that reveals the dependence of a property or activity on the whole molecular structure or a substructural fragment is called Quantitative Structure-Activity Relationship (QSAR). The development of QSAR models with good predictive capabilities is based on the effective transformation of structural features of molecules into numerical quantities. Topological indices (TI) are widely used as molecular descriptors in the construction of QSARs, and their derivatives such as Quantitative Structure-Property Relationships (QSPR) and Quantitative StructureToxicity Relationships (QSTR). For various applications of topological indices, we encourage our reader to consult references.[1–7]

The fourth atom bond connectivity index was introduced by Ghorbani and Hosseinzadeh,[8] in 2010. This index, based in the atom-bond connectivity (ABC) index previously published by Estrada et al.,[9] is defined as

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S(u) + S(v) - 2}{S(u)S(v)}},$$

where $S(u), S(v) \geq 1$ are integers. Here, $S(u)$ defined the degree sum of neighbour vertices that are connected to $u \in G$. The sum is extended for all the edges, that is, for each pair u,v that verifies $uv \in E(G)$. We encourage our reader to see references,[10–12] for further study of various types of atom bond connectivity index and results. In this paper, we concentrate on it and showed how it helps to predict the physicochemical properties of polycyclic aromatic hydrocarbons.

Methods

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. We use edge partition to compute the fourth atom bond connectivity index (ABC_4). The edge partition depends on the degree sum of neighbour vertices of the end vertices of edges. Based on the degree sum of neighbour vertices of the end vertices of each edge, the edge set can be partitioned into non-empty disjoint subsets. We have done the regression analysis by using Microsoft excel data analysis tools.

Results and Discussion

Significance of the fourth atom bond connectivity index

To consider a topological index as a descriptor of molecular structure it is necessary to test its ability to describe at least one physicochemical property of molecules. According to Milan Randić,[13] a good topological index must satisfy the following criteria:

1. have structural interpretation
2. have good correlation with at least one property
3. preferably discriminate among isomers

4. be locally defined
5. be generalizable to “higher" analogues
6. be preferably independent from other descriptors
7. be simple
8. not be based on properties
9. not be trivially related to other descriptors
10. be possible to construct efficiently
11. be based on familiar structural concepts
12. show a correct size dependence
13. change gradually with gradual change in structures

Some eminent researchers were considered various types of topological indices and tested their predictive ability of physicochemical properties of molecules in references.[10,14–17] In this paper, we considered 22 benzenoid hydrocarbons to test the predictive ability of the fourth atom bond connectivity index. The experimental data of benzenoid hydrocarbons are found at references[18–26] and https://pubchem.ncbi.nlm.nih.gov. The experimental data of benzenoid hydrocarbons are shown in Table 1. The fourth atom bond connectivity index of benzenoid hydrocarbons is shown in Table 2. Molecular graphs of benzenoid hydrocarbons are depicted in Figure 1. We have observed that the fourth atom bond connectivity index plays a vital role in predicting the boiling point (BP), molar entropy (S), acentric factor (ω), octanol-water partition coefficient (log$P$) and Kovats retention index (RI) of polycyclic aromatic hydrocarbons. The correlation coefficient (R) of the fourth atom bond connectivity index with some physicochemical properties of benzenoid hydrocarbons is shown in Table 3.

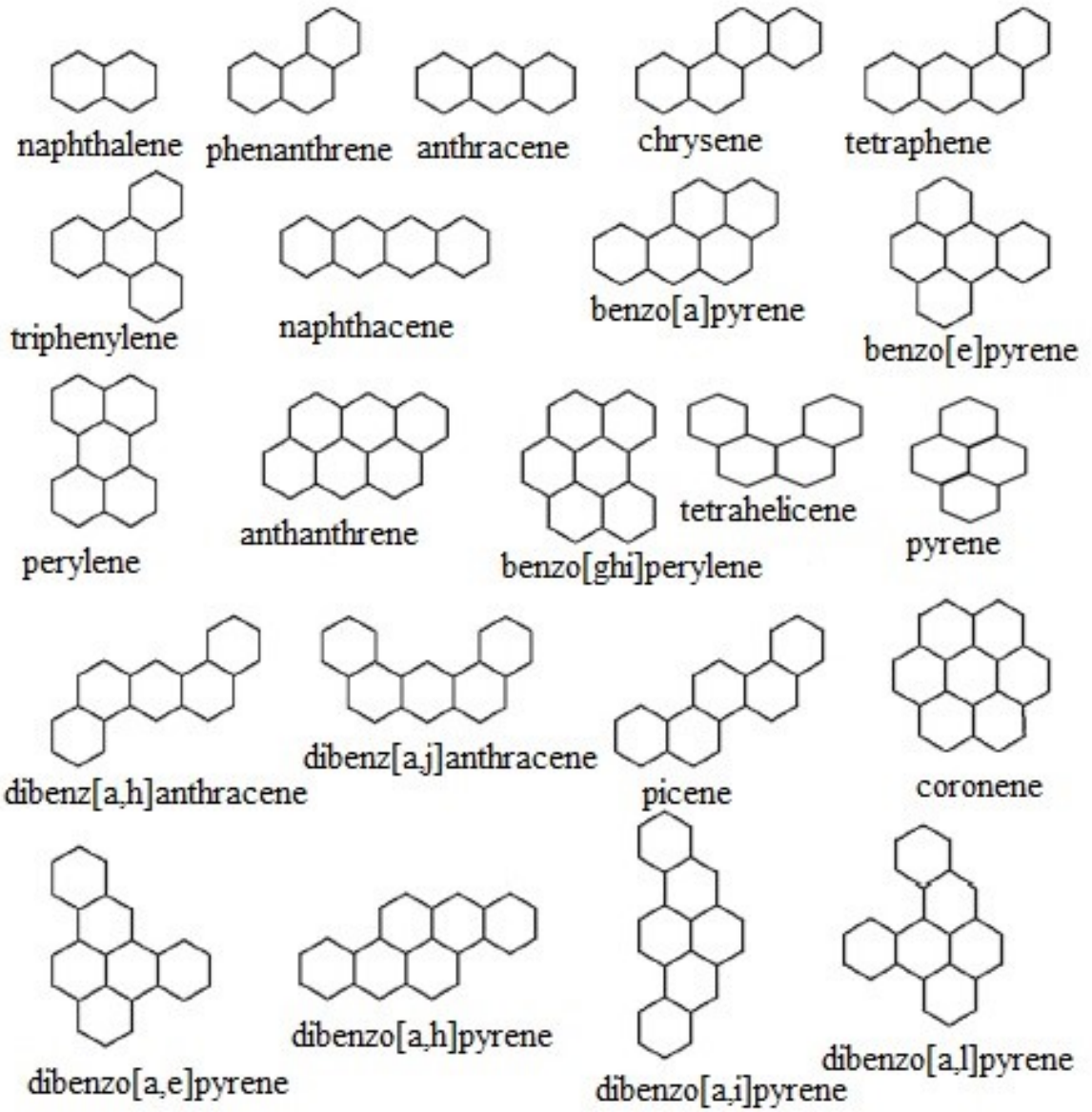


Figure 1: Molecular graphs of benzenoid hydrocarbons

Table 1: Experimental values of some physiochemical properties of benzenoid hydrocarbons

benzenoid hydrocarbons	Boiling Point (BP) (^0C)	Entropy (S) $(Cal/mol \cdot K)$	AcentFac (ω)	log$P$	Retention Index
naphthalene	218	79.38	0.302	3.3	200
phenanthrene	338	93.79	0.394	4.46	300
anthracene	340.05	92.43	0.402	4.45	301.69
chrysene	431	106.83	0.46	5.81	400
tetraphene	425	108.22	0.46	5.76	398.5
triphenylene	429	104.66	0.46	5.49	400
naphthacene	440	105.47	0.46	5.76	408.3
benzo[a]pyrene	496	111.85	–	6.13	453.44
benzo[e]pyrene	493	110.46	–	6.44	450.73
perylene	497	109.10	0.49	6.25	456.22
anthanthrene	547	114.10	–	7.04	503.89
benzo[ghi]perylene	542	114.10	–	6.63	501.32
dibenz[a,h]anthracene	536	119.87	–	6.75	495.45

dibenz[a,j]anthracene	531	119.87	–	6.54	489.8
picene	519	119.87	0.54	7.11	500
coronene	590	116.36	0.54	7.64	549.67
benzo[c]phenanthrene	448	113.61	–	5.7	391.12
pyrene	404	96.06	0.41	4.88	351.22
dibenzo[a,e]pyrene	592	124.89	–	7.28	551.53
dibenzo[a,h]pyrene	596	123.50	–	7.28	559.9
dibenzo[a,i]pyrene	594	123.50	–	7.28	556.47
dibenzo[a,l]pyrene	595	131.69	–	7.71	553

Table 2: Fourth atom bond connectivity index of benzenoid hydrocarbons

benzenoid hydrocarbons	ABC_4
naphthalene	6.224138
phenanthrene	8.7750922781
anthracene	8.7660753014
chrysene	11.3250008979
tetraphene	11.3153809443
triphenylene	11.3394347615
naphthacene	11.3080122236
benzo[a]pyrene	12.654264282
benzo[e]pyrene	12.6666592974
perylene	12.6725367047
anthanthrene	13.9828083547
benzo[ghi]perylene	13.9880064259
dibenz[a,j]anthracene	13.8646865871
picene	13.8749095177
coronene	15.303476147
benzo[c]phenanthrene	11.3263909473
pyrene	10.1040451613
dibenzo[a,e]pyrene	15.215230162
dibenzo[a,h]pyrene	15.204483026
dibenzo[a,i]pyrene	15.204483026
dibenzo[a,l]pyrene	15.217549156

Using the data in Table 1 and Table 2, linear regression models were obtained for boiling point (BP), molar entropy (S), acentric factor (ω), octanol water partition coefficient (log$P$), and Kovats retention index (RI). All correlation equations were internally validated by the leave-one-out method, and the corresponding Q-squares were calculated.

$$BP = -17.1079(\pm 9.742207) + 40.03475(\pm 0.7675)ABC_4 \quad (1)$$

$$N = 22, R^2 = 0.992703, S_e = 8.656109, F = 2720.895, SF = 7.57 \times 10^{-23}, Q^2 = 0.990363$$

$$S = 51.25735(\pm 4.186171) + 4.784723(\pm 0.329793)ABC_4 \quad (2)$$

$$N = 22, R^2 = 0.913228, S_e = 3.719481, F = 210.4902, SF = 4.44 \times 10^{-12}, Q^2 = 0.895739$$

$$\omega = 0.152754(\pm 0.018574) + 0.026756(\pm 0.00165)ABC_4 \quad (3)$$

$$N = 11, R^2 = 0.966925, S_e = 0.01315, F = 263.1126, SF = 5.71 \times 10^{-8}, Q^2 = 0.947018$$

$$\log P = 0.42869(\pm 0.194556) + 0.460467(\pm 0.015327)ABC_4 \quad (4)$$

$$N = 22, R^2 = 0.97832, S_e = 0.172866, F = 902.5277, SF = 4.08 \times 10^{-18}, Q^2 = 0.974667$$

$$RI = -43.1133(\pm 5.162788) + 39.09856(\pm 0.406732)ABC_4 \quad (5)$$

$$N = 22, R^2 = 0.997840, S_e = 4.587222, F = 9240.703, SF = 3.89 \times 10^{-28}, Q^2 = 0.997482$$

Where, N, R^2, S_e, F, SF and Q^2 denote the population, coefficient of determination, standard error of estimate, Fischer F-values, F-significance and cross-validation coefficient of determination, respectively. Using the regression models, we calculated the acentric factor (ω) of benzenoid hydrocarbons shown in Table 4. Scatter plot between the boiling point (BP), molar entropy (S), acentric factor (ω), octanol water partition coefficient ($\log P$), and Kovats retention index (RI) with the fourth atom bond connectivity index (ABC_4) are shown in Figure 2, Figure 3, Figure 4, Figure 5 and Figure 6 respectively.

Table 3: Correlation coefficients between the fourth atom bond connectivity index and some physiochemical properties of benzenoid hydrocarbons

Physicochemical properties benzenoid hydrocarbons	Correlation coefficient (R) with the fourth atom bond connectivity index (ABC_4)
Boiling Point (BP)	0.996345
Entropy (S)	0.95563
AcentFac (ω)	0.983324
Octanol Water Partition Coefficient ($\log P$)	0.989101
Retention Index (RI)	0.99892

Table 4: Acentric factors (ω) of benzenoid hydrocarbons

benzenoid hydrocarbons	AcentFac (ω) experimental	predicted
naphthalene	0.302	0.319
phenanthrene	0.394	0.387
anthracene	0.402	0.387
chrysene	0.46	0.456
tetraphene	0.46	0.456
triphenylene	0.46	0.456
naphthacene	0.46	0.455
benzo[a]pyrene	–	0.491
benzo[e]pyrene	–	0.492
perylene	0.49	0.492
anthanthrene	–	0.527
benzo[ghi]perylene	–	0.527
dibenz[a,h]anthracene	–	0.524
dibenz[a,j]anthracene	–	0.524
picene	0.54	0.524
coronene	0.54	0.562

benzo[c]phenanthrene	–	0.456
pyrene	0.41	0.423
dibenzo[a,e]pyrene	–	0.56
dibenzo[a,h]pyrene	–	0.56
dibenzo[a,i]pyrene	–	0.56
dibenzo[a,l]pyrene	–	0.56

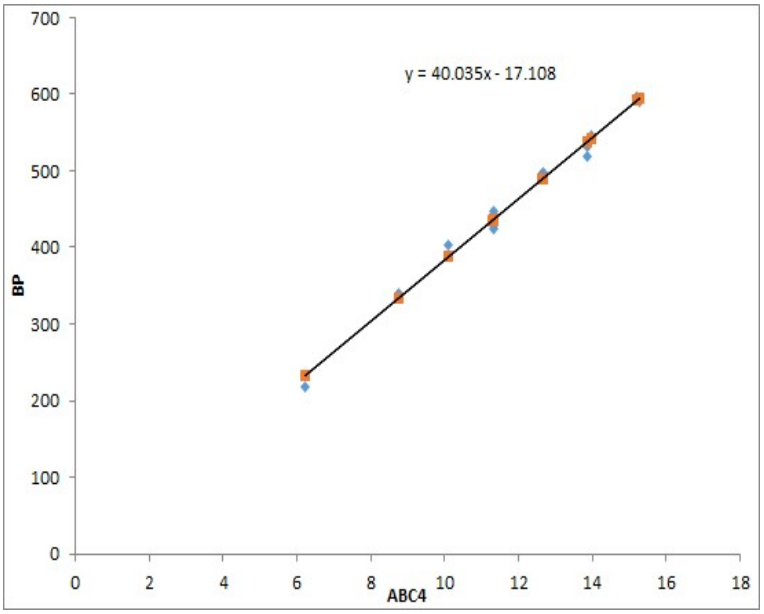


Figure 2: Scatter diagram of boiling point (*BP*) with the fourth atom bond connectivity index (ABC_4). Red dots: predicted y; blue dots: experimental y.

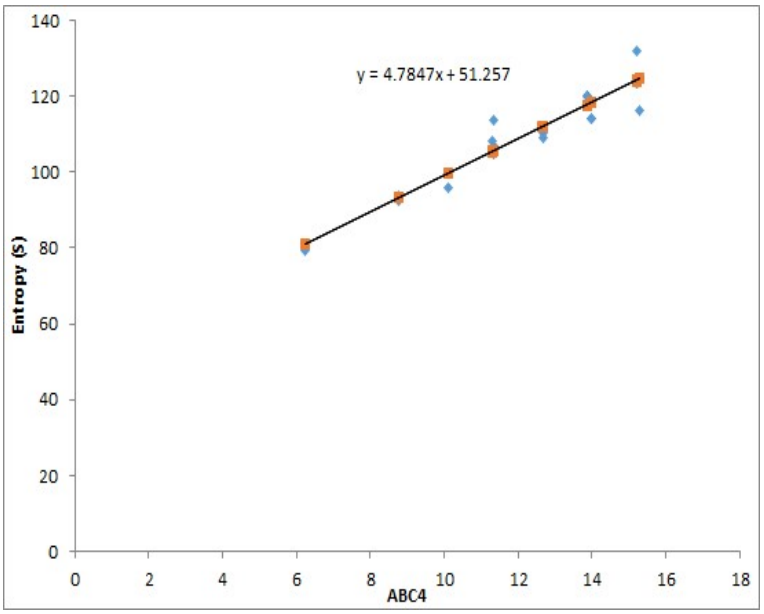


Figure 3: Scatter diagram of molar entropy (*S*) with the fourth atom bond connectivity index (ABC_4). Red dots: predicted y; blue dots: experimental y.

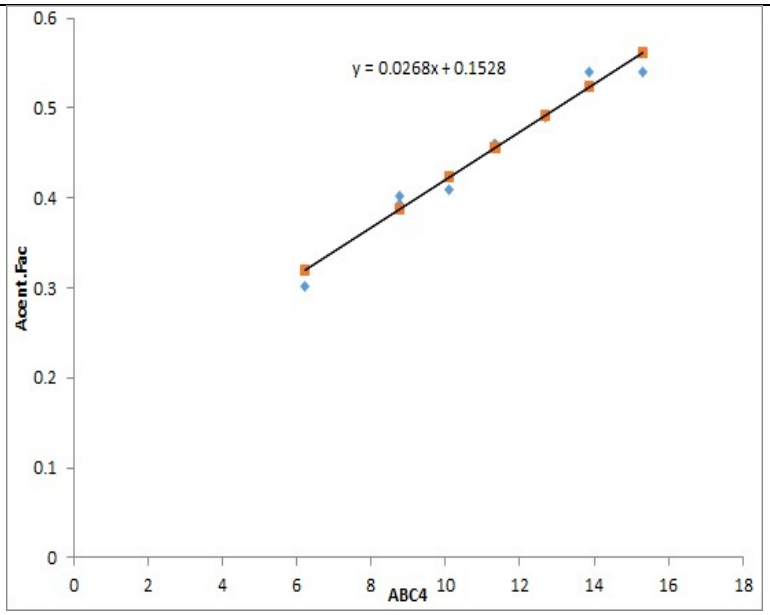


Figure 4: Scatter diagram of acentric factor (ω) with the fourth atom bond connectivity index (ABC_4). Red dots: predicted y; blue dots: experimental y.

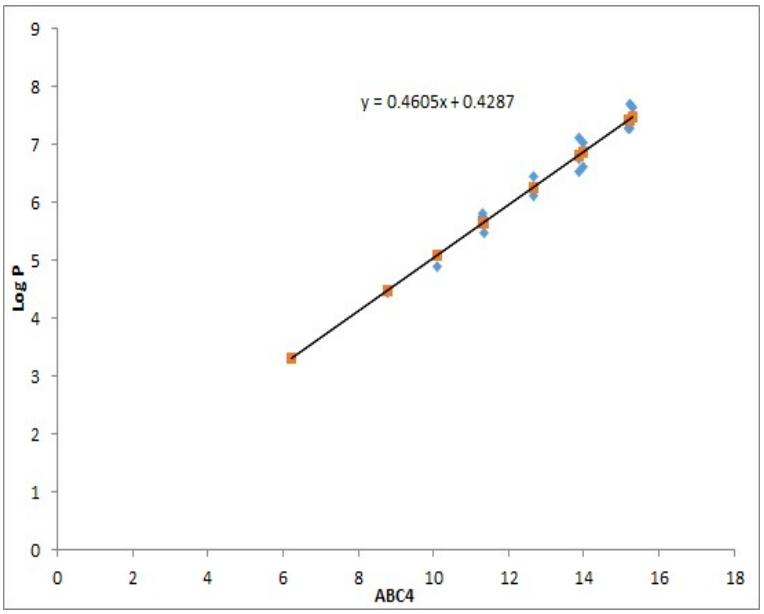


Figure 5: Scatter diagram of octanol-water partition coefficient (log$P$) with the fourth atom bond connectivity index (ABC_4). Red dots: predicted y; blue dots: experimental y.

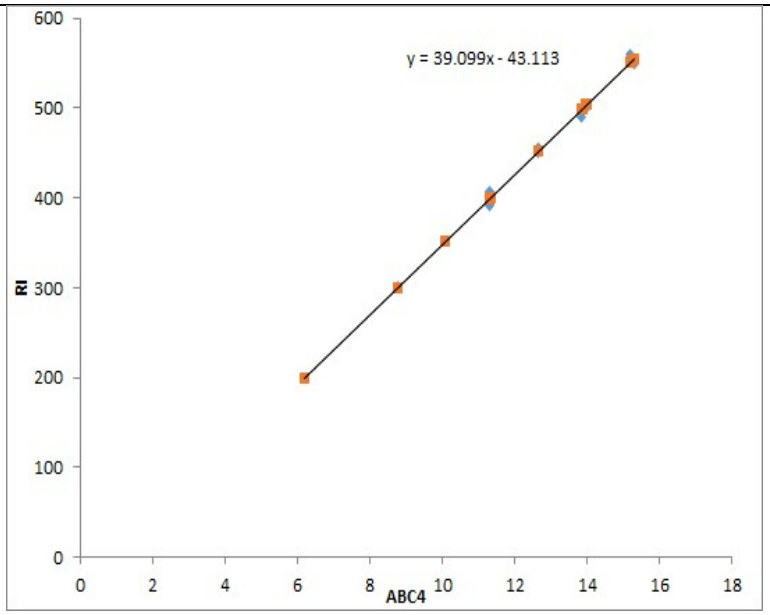


Figure 6: Scatter diagram of Kovats retention index (RI) with the fourth atom bond connectivity index (ABC_4). Red dots: predicted y; blue dots: experimental y.

The fourth atom bond connectivity index of hexagonal lattice networks

This section is devoted to the calculation of the connectivity index of the fourth atom of the hexagonal lattice. We noticed that the hexagonal lattice network is nothing but the union graph of hexagons. Some molecular structures are very similar to the hexagonal lattice network such as Graphene is an atomic-scale hexagonal lattice made of carbon atoms, hexagonal boron nitride (h-BN) is a layered material with a graphite-like structure in which planar networks of BN-hexagons are regularly stacked, the structure of the single-walled carbon nanotube is a regular hexagonal lattice whose vertices are the positions of the carbon atoms, hexagonal parallelogram nanotube and many more. First we defined a hexagon and a hexagonal lattice as a union graph of hexagons.

Definition 1 *(Hexagon). We defined a graph by* $\mathrm{H}(x,y) = (V,E)$*, for any* $x,y \in \mathrm{IR}$ *as follows:*

$$V = \{(x,y-2),(x+1,y-1),(x+1,y+1),$$
$$(x,y+2),(x-1,y+1),(x-1,y-1)\},$$

and

$$E = \Big\{\big((x,y-2),(x+1,y-1)\big),\big((x,y-2),(x-1,y-1)\big),\\ \big((x+1,y-1),(x+1,y+1)\big),\big((x+1,y+1),(x,y+2)\big),\\ \big((x,y+2),(x-1,y+1)\big),\big((x-1,y+1),(x-1,y-1)\big)\Big\}.$$

We note that each edge of H(x,y) are shared by H(x+1,y+3), H(x−1,y+3), H(x−1,y−3), H(x + 1,y − 3), H(x + 2,y), and H(x − 2,y), respectively. Therefore we can consider the hexagonal lattice network as a union graph of some H(x,y)'s. For example in this paper we defined a hexagonal lattice network HL[4,4] as follows:

$$\begin{aligned}\mathrm{HL}[4,4] = {} & \mathrm{H}(0,0)\cup\mathrm{H}(2,0)\cup\mathrm{H}(4,0)\cup\mathrm{H}(6,0)\\ & \cup\mathrm{H}(1,3)\cup\mathrm{H}(3,3)\cup\mathrm{H}(5,3)\cup\mathrm{H}(7,3)\\ & \cup\mathrm{H}(2,6)\cup\mathrm{H}(4,6)\cup\mathrm{H}(6,6)\cup\mathrm{H}(8,6)\\ & \cup\mathrm{H}(3,9)\cup\mathrm{H}(5,9)\cup\mathrm{H}(7,9)\cup\mathrm{H}(9,9).\end{aligned}$$

The example of an HL[4,4] and HL[m,n] is shown in Figure 7 and Figure 8 respectively. The edge partition of the hexagonal lattice network HL[m,n] with respect to the degree sum of neighbour vertices of the end vertices of each edge of HL[m,n] is shown in Table 5. Let us denote HL[m,n] as G_1.

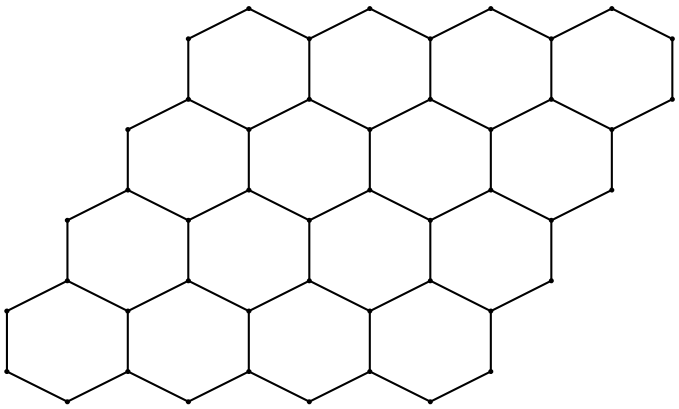
Theorem 1 *The fourth atom bond connectivity index ABC_4 of hexagonal lattice network G_1 is given by,*

$$\begin{aligned}ABC_4(G_1) = {} & 4\sqrt{\frac{7}{20}}+\frac{2\sqrt{8}}{5}+8\sqrt{\frac{2}{7}}+4(m+n-4)\sqrt{\frac{11}{42}}\\ & +2(m+n-2)\sqrt{\frac{2}{9}}+\frac{4(3mn-4m-4n+5)}{9}.\end{aligned} \quad (6)$$

Table 5: The edge partitions with respect to degree sum of neighbour vertices of end vertices of every edge of G_1

($S(u)$,$S(v)$) : $uv \in E(G_1)$	Total number of edges
(4,5)	4
(5,5)	2
(5,7)	8
(6,7)	4(m + n − 4)
(7,9)	2(m + n − 2)

(9,9)	$(m-2)(n-1)+(m-1)(2n-3)$

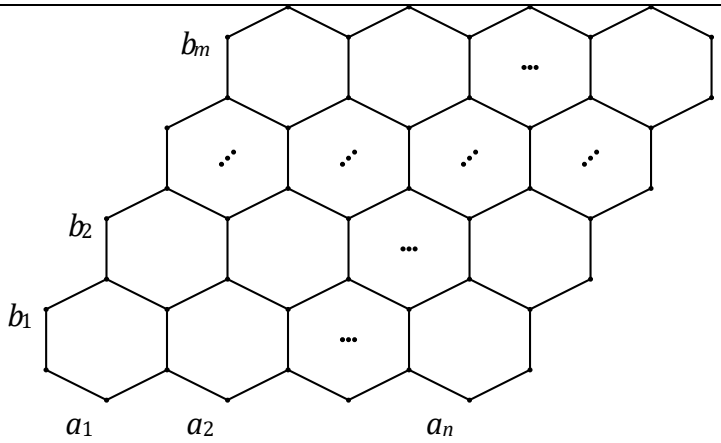


HL [4, 4]

Figure 7: The example of hexagonal lattice with 4 rows and 4 column

Proof. From the definition of the fourth atom bond connectivity index, we get

$$\begin{aligned} ABC_4(G_1) &= \sum_{uv\in E(G_1)}\sqrt{\frac{S(u)+S(v)-2}{S(u)S(v)}} \\ &= \sum_{uv\in E_1(G_1)}\sqrt{\frac{4+5-2}{4\cdot 5}}+\sum_{uv\in E_2(G_1)}\sqrt{\frac{5+5-2}{5\cdot 5}} \\ &\quad +\sum_{uv\in E_3(G_1)}\sqrt{\frac{5+7-2}{5\cdot 7}}+\sum_{uv\in E_4(G_1)}\sqrt{\frac{6+7-2}{6\cdot 7}} \\ &\quad +\sum_{uv\in E_5(G_1)}\sqrt{\frac{7+9-2}{7\cdot 9}}+\sum_{uv\in E_6(G_1)}\sqrt{\frac{9+9-2}{9\cdot 9}} \\ &= |E_1(G_1)|\Big(\sqrt{\frac{4+5-2}{4\cdot 5}}\Big)+|E_2(G_1)|\Big(\sqrt{\frac{5+5-2}{5\cdot 5}}\Big) \\ &\quad +|E_3(G_1)|\Big(\sqrt{\frac{5+7-2}{5\cdot 7}}\Big)+|E_4(G_1)|\Big(\sqrt{\frac{6+7-2}{6\cdot 7}}\Big) \\ &\quad +|E_5(G_1)|\Big(\sqrt{\frac{7+9-2}{7\cdot 9}}\Big)+|E_6(G_1)|\Big(\sqrt{\frac{9+9-2}{9\cdot 9}}\Big) \\ &= 4\Big(\sqrt{\frac{4+5-2}{4\cdot 5}}\Big)+2\Big(\sqrt{\frac{5+5-2}{5\cdot 5}}\Big)+8\Big(\sqrt{\frac{5+7-2}{5\cdot 7}}\Big) \\ &\quad +4(m+n-4)\Big(\sqrt{\frac{6+7-2}{6\cdot 7}}\Big)+2(m+n-2)\Big(\sqrt{\frac{7+9-2}{7\cdot 9}}\Big) \\ &\quad +(3mn-4m-4n+5)\Big(\sqrt{\frac{9+9-2}{9\cdot 9}}\Big). \end{aligned}$$



HL[m,n]

Figure 8: The example of hexagonal lattice network with *m* rows and *n* column

Hence follows the desired result as shown in equation 6.

Corollary 1 *For some different values of m and n, in the following corollary we calculate the fourth atom bond connectivity index of hexagonal lattice network by using equation 6.*

$$
\begin{aligned}
(i)\ ABC_4(\mathrm{HL}[1,4]) &= 11.31614,\\
(ii)\ ABC_4(\mathrm{HL}[1,5]) &= 13.86157,\\
(iii)\ ABC_4(\mathrm{HL}[2,3]) &= 13.98280,\\
(iv)\ ABC_4(\mathrm{HL}[2,4]) &= 17.86157,\\
(v)\ ABC_4(\mathrm{HL}[2,5]) &= 21.74033,\\
(vi)\ ABC_4(\mathrm{HL}[3,4]) &= 24.407,\\
(vii)\ ABC_4(\mathrm{HL}[4,4]) &= 30.95243,\\
(viii)\ ABC_4(\mathrm{HL}[5,4]) &= 37.49786,\\
(ix)\ ABC_4(\mathrm{HL}[5,5]) &= 45.37662.
\end{aligned}
$$

Using Corollary 1, for some particular values of *m* and *n* we predicted some physiochemical properties of hexagonal lattice network such as boiling point, molar entropy, acentric factor, octanol-water partition coefficient, Kovats Retention index shown in Table 6.

Table 6: Physiochemical properties (predicted) of hexagonal lattice networks for some particular values of *m* and *n*

(m,n)	Boiling Point (BP) (^0C)	Entropy (S) $(Cal/mol \cdot K)$	AcentFac (ω)	$\log P$	Retention Index (RI)
$(1,4)$ or naphthacene	435.93366	105.40133	0.456	5.63978	399
$(1,5)$ or pentacene	537.83995	117.58045	0.524	6.81195	499
$(2,3)$ or anthanthrene	542.69339	118.16050	0.527	6.86777	503
$(2,4)$ or $C_{28}H_{14}$	697.97995	136.71925	0.631	8.65395	655
$(2,5)$ or $C_{34}H_{16}$	853.26611	155.27795	0.735	10.44012	807
$(3,4)$	960.02	168.03	0.806	11.66	911
$(4,4)$	1222.07	199.35	0.982	14.68	1167
$(5,4)$	1484.11	230.67	1.15	17.69	1423
$(5,5)$	1799.54	268.37	1.36	21.32	1731

Conclusions

In this paper, we deal with the fourth atom bond connectivity index and showed how it helps to predict the physicochemical properties of polycyclic aromatic hydrocarbons. We computed the fourth atom bond connectivity index of hexagonal lattice networks. Based on our regression models, we predicted some physicochemical properties of hexagonal lattice networks for some particular values of *m* and *n*. We also calculated the acentric factor of some benzenoid hydrocarbons by using our models. We hope this study, will help the researchers for further application, for example, to the characterization of nanotubes and graphene structures.

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References

(1) Mekenyan, O.; Bonchev, D.; Sabljic, A.; Trinajstić, N. Applications of Topological Indices to QSAR. The Use of the Balaban Index and the Electropy Index for Correlations with Toxicity of Ethers on Mice. *Acta Pharmaceutica Jugoslavica* 1987, *37*, 75–86.

(2) Pyka, A. Application of topological indices for prediction of the biological activity of selected alkoxyphenols. *Acta Poloniae Pharmaceutica* 2002, *59*, 347–352.

(3) Estrada, E.; Uriarte, E. Recent advances on the role of topological indices in drug discovery research. *Current Medicinal Chemistry* 2001, *8*, 1573–1588.

(4) Garcia-Domenech, R.; de Julian-Ortiz, J.; Duart, M.; Garcia-Torrecillas, J.; AntonFos, G.; Rios-Santamarina, I.; Gregorio-alapont, C. D.; Galvez, J. Search of a topological pattern to evaluate toxicity of heterogeneous compounds. *SAR and QSAR in Environmental Research* 2001, *12*, 237–254.

(5) Randić, M. Characterization of molecular branching. *Journal of the American Chemical Society* 1975, *97*, 6609–6615.

(6) Natarajan, R.; Kamalakanan, P.; Nirdosh, I. Applications of topological indices to structure-activity relationship modelling and selection of mineral collectors. *Indian Journal of Chemistry. Section A: Inorganic, Physical, Theoretical & Analytical* 2003, *42*, 1330–1346.

(7) Basak, S. C.; Mills, D.; Gute, B. D.; Grunwald, G. D.; Balaban, A. T. *Topology in Chemistry*; Elsevier, 2002; pp 113–184.

(8) Ghorbani, M.; Hosseinzadeh, M. A. Computing ABC4 index of nanostar dendrimers. *Optoelectronics and Advanced Materials-Rapid Communications* 2010, *4*, 1419–1422.

(9) Estrada, E.; Torres, L.; Rodriguez, L.; Gutman, I. An atom-bond connectivity index: modelling the enthalpy of formation of alkanes. *Indian Journal of Chemistry. Section A: Inorganic, Physical, Theoretical & Analytical* 1998, *37A*, 849–855.

(10) Gutman, I.; Tošović, J.; Radenković, S.; Marković, S. On atom-bond connectivity index and its chemical applicability. *Indian Journal of Chemistry* 2012, *51*, 690–694.

(11) Xing, R.; Zhou, B.; Dong, F. On atom–bond connectivity index of connected graphs. *Discrete Applied Mathematics* 2011, *159*, 1617–1630.

(12) Shao, Z.; Wu, P.; Zhang, X.; Dimitrov, D.; Liu, J.-B. On the maximum ABC index of graphs with prescribed size and without pendent vertices. *IEEE Access* 2018, *6*, 27604–27616.

(13) Randić, M. Generalized molecular descriptors. *Journal of Mathematical Chemistry* 1991, *7*, 155–168.

(14) Gutman, I.; Tošović, J. Testing the quality of molecular structure descriptors. Vertexdegree-based topological indices. *Journal of the Serbian Chemical Society* 2013, *78*, 805–810.

(15) Hosoya, H. Chemical meaning of octane number analyzed by topological indices. *Croatica Chemica Acta* 2002, *75*, 433–445.

(16) Ramane, H. S.; Yalnaik, A. S. Status connectivity indices of graphs and its applications to the boiling point of benzenoid hydrocarbons. *Journal of Applied Mathematics and Computing* 2017, *55*, 609–627.

(17) Mondal, S.; De, N.; Pal, A. QSPR analysis of some novel neighborhood degree based topological descriptors. *Complex & Intelligent Systems* 2019,

(18) Alvarez, V. H.; Saldana, M. D. Modeling solubility of polycyclic aromatic compounds in subcritical water. *Industrial & Engineering Chemistry Research* 2011, *50*, 11396–11405.

(19) Alberty, R. A.; Chung, M. B.; Reif, A. K. Standard chemical thermodynamic properties of polycyclic aromatic hydrocarbons and their isomer groups. III. Naphthocoronene series, ovalene series, and first members of some higher series. *Journal of Physical and Chemical Reference Data* 1990, *19*, 349–370.

(20) Alberty, R. A.; Chung, M. B.; Reif, A. K. Standard chemical thermodynamic properties of polycyclic aromatic hydrocarbons and their isomer groups. II. Pyrene series, naphthopyrene

series, and coronene series. *Journal of Physical and Chemical Reference Data* 1989, *18*, 77–109.

(21) Alberty, R. A.; Reif, A. K. Standard chemical thermodynamic properties of polycyclic aromatic hydrocarbons and their isomer groups I. Benzene series. *Journal of Physical and Chemical Reference Data* 1988, *17*, 241–253.

(22) Alberty, R. A.; Reif, A. K. Erratum: Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups I. Benzene Series [J. Phys. Chem. Ref. Data 1 7, 241 (1988)]. *Journal of Physical and Chemical Reference Data* 1989, *18*, 551–553.

(23) Wang, H.; Frenklach, M. Transport properties of polycyclic aromatic hydrocarbons for flame modeling. *Combustion and Flame* 1994, *96*, 163–170.

(24) Wang, Q.; Jia, Q.; Ma, P. Prediction of the acentric factor of organic compounds with the positional distributive contribution method. *Journal of Chemical & Engineering Data* 2012, *57*, 169–189.

(25) Perry, M.; White, C. Correlations of molecular connectivity with critical volume and acentricity. *AIChE journal* 1987, *33*, 146–151.

(26) White, C. M. Prediction of the boiling point, heat of vaporization, and vapor pressure at various temperatures for polycyclic aromatic hydrocarbons. *Journal of Chemical & Engineering Data* 1986, *31*, 198–203.

(27) Vasilyev, A.; Stevanovic, D. MathChem: a Python package for calculating topological indices. *MATCH Communications in Mathematical and in Computer Chemistry* 2014, *71*, 657–680.