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A Significant Computation for Finding the PI index of Phenylene

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Abstract

PI indices for linear Phenylene are obtained by a significant method by considering its edges in various directions and their corresponding number of parallel edges in their molecular graph. In this paper, we obtained the PI index for linear Phenylene for various cases and different structures. The corresponding indices are derived as formulas and also the inferences are tabulated and the values are compared with its structures.

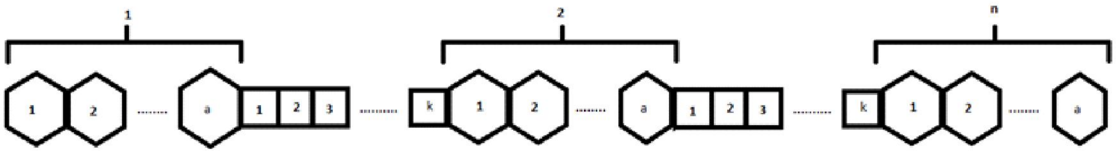
Key words: Molecular Graph, Phenylene, M-Polynomial, Topological indices.

Introduction

Chemical Graph Theory is an interdisciplinary science that applies Graph Theory to the study of molecular structures. The molecules or chemical compounds are modeled by an undirected graph. Chemistry produces the objects of its own study and chemical composition is a unifying concept for all the experimental sciences. “There are no restrictions on the design of structural invariants; the limiting factor is one’s own imagination.”[1]. Molecular structure is one of the most fruitful scientific concepts of this century. In the molecular graph the vertices represent atoms or group of atoms and edges represent chemical bonds between atoms or group of atoms.[2] The molecular descriptor is the final result of a logic and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment[3-5]. The basic assumptions are that different molecular structures have different chemical properties and similar molecular structures have similar molecular properties. Each molecular representation represents a different way to look at the molecular structure and its chemical meaning is strongly immersed in the framework of the chemical theories[6]. A topological index is a numerical parameter mathematically derived from the graph structure. It is a graph invariant thus it does not depend on the labeling or pictorial representation of the graph. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity (e.g., pharmacology)[7-9]. several applications of the PI index are reported in the literature[10-13]. Many methods for the calculation of PI indices of some systems are reported in[14-20]. In this paper, we calculated the PI index of linear Phenylene using a significant and easier method compared to the previous methods in the literature.

1. Linear Phenylene :

Linear phenylene contains ‘an’ number of hexagons, ‘a(n-1)’ number of squares, ‘a’ represent the number of squares in each segment, k represents the number of squares in each segment, n represents the number of segments in the structure of phenylene. Therefore, the linear phenylene can be denoted as G (a,k,n) and its graphical structure is explained below.



Definition of PI Index: The PI index of a graph G is defined as, $PI(G)=\sum[n_1(e)+n_2(e)]$ where for edge e = xy, $n_1(e)$ is the number of edges of G lying closer to x than y, $n_2(e)$ is the number of edges of G lying closer to y than x and summation goes over all edges of G. The edges equidistant from x and y are not considered for the calculation of PI index.

Linear Phenylene for a=1 :

Here, we considered the case that a = k = 1 and also we observed that ‘a’ and ‘k’ are equal for $n \geq 2$ in the structure of phenylene but if n = 1 then a = 1 and k = 0. We can say that the number of edges for linear phenylene is e = 8n-2 for all n.

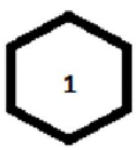


Figure: 1Graph of G(1,0,1)

Table 1. Calculation for the PI index for n=1

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	S * N_p	PI Index
Vertical	2	1	2	2(e-2)
Horizontal	0	0	0	0
Slanting	2	2	4	4(e-2)
PI index				6(e-2)

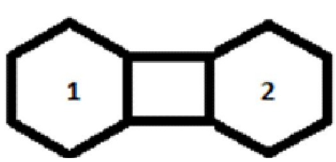


Figure: 2 Graph ofG(1,1,2)

Table 2. Calculation for the PI index for n=2

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	S * N_p	PI Index
Vertical	4	1	4	4(e-4)
Horizontal	2	1	2	2(e-2)
Slanting	2	4	8	8(e-2)
PI index				10(e-2)+ 4(e-4)

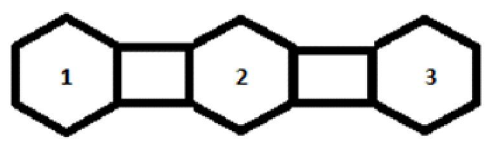


Figure: 3 Graph of G(1,1,3)

Table 3. Calculation for the PI index for n=3

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	S * N_p	PI Index
Vertical	6	1	6	4(e-4)
Horizontal	2	2	4	4(e-2)
Slanting	2	6	12	12(e-2)
PI index				16(e-2)+ 4(e-4)

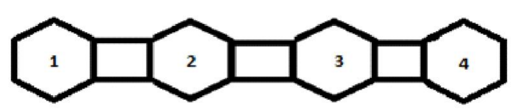


Figure: 4 Graph of G(1,1,4)

Table 4. Calculation for the PI index for n=4

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	$S * N_p$	PI Index
Vertical	8	1	8	8(e-8)
Horizontal	2	3	6	6(e-2)
Slanting	2	8	16	16(e-2)
		PI index		22(e-2)+ 8(e-8)

In Vertical Direction, for n = 1,2,3,4… , product is 2,4,6,8 … respectively. Then the general Term is given by 2n. Therefore, the PI Index can becalculated as 2n(e-2n). In Horizontal Direction, for n = 1,2,3,4…, Product is 0,2,4,6 … respectively. Then the general Term is given by 2n-2 . Therefore, the PI Index can be calculated as (2n-2)(e-2). In Slanting Direction, for n = 1,2,3,4…,Product is 4,8,12,16 … respectively. Then the general Term is 4n. Therefore the PI Index is 4n(e-2). For n=1,2,3,4… and a=1.

The PI Index of $G(a,k,n) = 2n(e-2n)+(2n-2)(e-2)+4n(e-2)$,

$= 2ne-4n^2 +2ne – 2e - 4n +4 +4ne – 8n$

$= 8ne – 12n – 4n^2 + 4 – 2e$

$= 8n(8n-2) – 12n – 4n^2 + 4 – 2(8n - 2)$

$= 64n^2 – 16n – 12n – 4n^2 + 4–16n + 4$

$=$ $\mathbf{60n^2–44n + 8}$ for a=1 and for all 'n'.

Linear Phenylene for a=2 :

Here, we consider the case that a = 2 and also we observed that 'a' and 'k' are equal for $n \geq 2$ in the structure of phenylene but if n=1 then a=2 and k=0. We can say that the number of edges for linear phenylene is e = 16n-5 for all n.

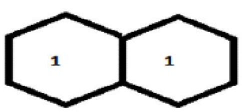


Figure: 5 Graph of G(2,0,1)

Table 5. Calculation for the PI index for a=2,n=1

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	$S * N_p$	PI Index
Vertical	3	1	3	3(e-3)
Horizontal	0	0	0	0
Slanting	2	4	8	8(e-2)
		PI index		8(e-2)+ 3(e-3)

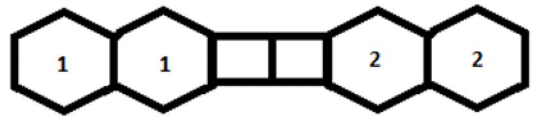


Figure: 6 Graph of G(2,2,2)

Table 6. Calculation for the PI index for a=2,n=2

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	$S * N_p$	PI Index
Vertical	7	1	7	7(e-7)
Horizontal	2	2	4	4(e-2)
Slanting	2	8	16	16(e-2)
		PI index		20(e-2)+ 7(e-7)

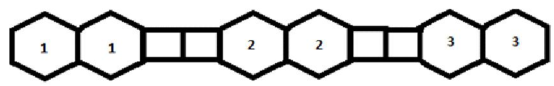


Figure: 7 Graph of G(2,2,3)

Table 7 Calculation for the PI index for a=2,n=3

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	$S * N_p$	PI Index
Vertical	11	1	11	11(e-11)
Horizontal	2	4	8	8(e-2)
Slanting	2	12	24	24(e-2)
		PI index		32(e-2)+ 11(e-11)

In Vertical Direction, for n = 1,2,3… , product is 3,7,11 … respectively. Then the general Term is given by 4n-1. Therefore, the PI Index can be calculated as (4n-1)(e-4n+1). In Horizontal Direction, for n = 1,2,3…, Product is 0,4,8 … respectively. Then the general Term is given by 4n-4 . Therefore, the PI Index can be calculated as (4n-4)(e-2). In Slanting Direction, for n = 1,2,3,4…,Product is 8,16,24… respectively. Then the general Term is 4n. Therefore the PI Index is 8n(e-2). For n=1,2,3… and a=2.

The PI Index of G(a,k,n) $=(4n-1)(e-4n+1)+(4n-4)(e-2)+8n\ (e-2)$

$=(4n-1)(16n-5-4n+1)+(4n-4)(16n-5-2)+8n\ (16n-5-2)$

$= (4n-1)(12n-4)+(4n-4)(16n-7)+8n(16n-7)$

$=48n^2 – 28n+4 +64n^2-92n-28 +128n^2 – 56n$

$= 240n^2 - 176n – 32$ *for a=2 and for all 'n'.*

Linear Phenylene for a=3 :

Linear phenylene contains n number of hexagons and n-1 squares. So we can say that the number of edges for linear phenylene is e = 24n-8. Phenylene can be denoted as G(a,k,n) where a represents the number of squares in each segment, k represents the number of squares in each segment, n represents the number of segments in the structure of phenylene. Therefore, the linear phenylene can be denoted as G(3,k,n).

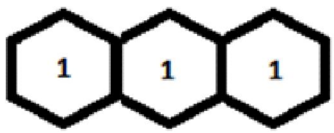


Figure 8 Graph of G(3,0,1)

Table 8. Calculation for the PI index for a=3,n=1

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	$S * N_p$	PI Index
Vertical	4	1	4	4(e-4)
Horizontal	0	0	0	0
Slanting	2	6	12	12(e-2)
PI index				12(e-2)+ 4(e-4)

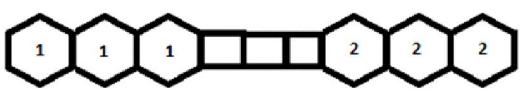


Figure: 9 Graph of G(3,3,2)

Table 9. Calculation for the PI index for a=3,n=2

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	$S * N_p$	PI Index
Vertical	10	1	10	10(e-10)
Horizontal	2	3	6	6(e-2)
Slanting	2	12	24	24(e-2)
PI index				30(e-2)+ 10(e-10)

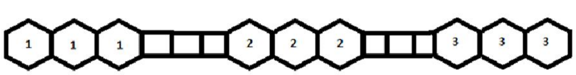


Figure: 10 Graph of G(3,3,3)

Table 10. Calculation for the PI index for a=3,n=3

Direction of parallel edges	No. of parallel edges (N_p)	Set of edges (S)	$S * N_p$	PI Index
Vertical	16	1	16	16(e-16)
Horizontal	2	6	12	12(e-2)
Slanting	2	18	36	36(e-2)
PI index				48(e-2)+ 16(e-16)

In Vertical Direction, for n = 1,2,3,4… , product is 4,10,16 … respectively. Then the general Term is given by 6n-2. Therefore, the PI Index can be calculated as (6n-2)(e-(6n-2)). In Horizontal Direction, for n = 1,2,3,4…, Product is 0,6,12 … respectively. Then the general Term is given by 6n-6 . Therefore, the PI Index can be calculated as (6n-6)(e-2). In Slanting Direction, for n = 1,2,3,4…,Product is 12,24,36 … respectively. Then the general Term is 12n. Therefore the PI Index is 12n(e-2). For n=1,2,3,4… and a=1.

The PI Index
of G(3,k,n) = (6n-2)(e-(6n-2))+(6n-6)(e-2)+12n (e-2)
= (6n-2)(24n-8-6n+2)+(6n-6)(e-2)12n(24n-8-2)
= (6n-2)(18n-6)+(6n-6)(e-2)+12n(24n-10)
= $108n^2$ –72n12+(6n-6)(24n-8-2)+12n(24n-10)
= $108n^2$–72n+12+$144n^2$-204n+60+$288n^2$-120n
= $540n^2$ – 396n +72for a=3 and for all ‘n’.

PI index for Linear Phenylene for any values of ‘a’ and ‘n’:

In Vertical Direction, for a= 1,2,3… , Product is 2n, 4n-1, 6n-2 … respectively. Then the general Term is given by a(2n-1) + 1. Therefore, the PI Index can be calculated as [a(2n-1)+1] (e –(a(2n-1)+1)). In Horizontal Direction, for a= 1,2,3… Product is 2n-2,4n-4, 6n-6 … respectively. Then the general Term is given by 4na(e - 2). Therefore, the PI Index can be calculated as (6n-6)(e-2). In Slanting Direction, for a= 1,2,3…, Product is 4n, 8n, 12n … respectively. Then the general Term is 4na. Therefore the PI Index is 2a(n-1)(e - 2). For a= 1,2,3…,the number of edges ‘e’ is given by 8n-2,16n-5,24n-8….Hence, the general term for the number of edges ‘e’ for any ‘a’ is given by (8n-3)a+1.

PI index for G(a,k,n)
= [a(2n-1)+1] (e–(a(2n-1)+1))+[4na] (e-2)+[2a(n-1)](e - 2)
= [a(2n-1)+1] [(8n – 3)a+1 – (a(2n-1)+1))+[4na]((8n – 3)a+1 – 2)+[2a(n-1)] (8n – 3)a+1 – 2)
= {(2na – a + 1)(8na – 3a +1) – (2na – a + 1)}+{(2na – 2a)(8na -3a -1)}+{(4na)(8na – 3a -1)}
={(2na – a +1)(8na – 3a +1–2na +a –1)}+{(2na – 2a)(8na - 3a -1)}+{$32n^2a^2$ – $12na^2$ – 4na}
= $60n^2a^2$ – $44na^2$ +$8a^2$for all values of a and n.

Inferences :

For a = 1,2,3 PI indices are calculated as polynomials as $60n^2 - 44n + 8$, $240n^2 - 176n + 32$, $540n^2 - 396n + 72$ respectively where 'a' represents the number of squares in each segment, n represents the number of segments in the structure of phenylene. PI indices can be obtained easily from the polynomial $60n^2a^2 - 44na^2 + 8a^2$ for any values of 'a' and 'n'.

Table 11. PI indices for G(a,k,n)

a	k	N	PI[G(a,k,n)]	a	k	n	PI[G(a,k,n)]	a	k	n	PI[G(a,k,n)]
1	0	1	24	2	0	1	32	3	0	1	216
1	1	2	160	2	2	2	576	3	2	2	1440
1	1	3	416	2	2	3	1600	3	2	3	3744
1	1	4	792	2	2	4	3104	3	2	4	7128
1	1	5	1288	2	2	5	5088	3	2	5	11592

Conclusion and Future Study

Several scientists are involved in searching for new molecular descriptors able to catch new aspects of the molecular structure. This kind of research involves creativity and imagination together with solid theoretical basis allowing obtaining numbers with some structural chemical meaning. These results can be programmable by any language in computer science and numerically determinable by software. Thus, Mathematical chemistry will pave a way to structural analysis of chemicals.

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