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M-Polynomials of Penta-chains

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Abstract

Using the vertex degrees of the graphs, M- polynomials of several types of graphs consisting of concatenated pentagonal rings are obtained and studied in this paper. The vertex degree based indices like Randic, Geometric – Arithmetic, Sum Connectivity, Harmonic, First Zagreb, Second Zagreb, Second Modified Zagreb, Inverse Sum, Alberston, Atom – bond Connectivity, Symmetric – Division index and Augmented Zagreb indices etc., of penta-chains can be calculated easily by using the proposed M-Polynomials of the penta-chains for single, alternating and double-row penta-chains of two types.

Key words: M-Polynomial, Topological indices, Molecular graph, Penta-chain.

Introduction

In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound[1]. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure.[2] Topological descriptors are derived from hydrogen-suppressed molecular graphs, in which the atoms are represented by vertices and the bonds by edges. The connections between the atoms can be described by various types of topological matrices (e.g., distance or adjacency matrices), which can be mathematically manipulated so as to derive a single number, usually known as graph invariant, graph-theoretical index or topological index.[3,4] As a result, the topological index can be defined as two-dimensional descriptors that can be easily calculated from the molecular graphs, and do not depend on the way the graph is depicted or labeled and no need of energy minimization of the chemical structure.

M-Polynomial of graph G :

If $G = (V, E)$ is a graph and $v \in V$, then $d_v(G)$ (or d_v for short if G is clear from the context) denotes the degree of v. Let G be a graph and let $m_{ij}(G), i, j \geq 1,$ be the number of edges e = uv of G such that $\{d_u(G), d_v(G)\} = \{i, j\}$.

The M-polynomial of G as $M(G;x,y)=\sum_{i\le j} m_{ij}(G)x^i y^j$. For a graph $G=(V,E)$, a degree-baijsed topological index is a graph invariant of the form $I(G)=\sum_{e=uv\in E} f(d_u,d_v)$ where $f=f(x,y)$ is a function appropriately selected for possible chemical applications.

The popular vertex degree based topological indices are taken from literature and tabulated for futher calculation of indices for any graph $G=(V,E)$ of their edges e = uv, where 'i' represents $d_u(G)$ and 'j' represents $d_v(G)$ and

$$\{\varphi_{ij}\}=\sum_{e=uv\in G} f(i,j)$$

Straight Chaining of Pentagons [SCP] :

A straight chaining is a graph consisting of n pentagonal rings, every two successive rings have a common edge, forming a chain denoted by SCP(n), where 'n' denotes the number of pentagons in that chain.

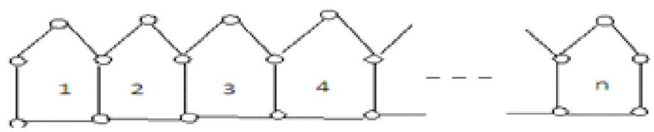

Figure 1. SCP

The number of edges are calculated for the various combinations of i,j and also for the number of pentagons n=1,2,3,4,5 from the graph of SCP in figure 1 and the results are tabulated below:

i,j	n=1	n=2	n=3	n=4	n=5
2,2	2	2	2	2	2
2,3	0	4	4	4	4
3,3	0	1	5	9	13

If SCP(n) is the straight chain of pentagons, $n\ge 1$, n represents the number of pentagons in SCP(n), then the M-Polynomial of straight chain of pentagons is

$$\mathrm{M(SCP[n;\, x, y])}=\begin{cases}5x^2y^2, n=1\\ 4x^2y^2+4x^2y^3+(4n-7)x^3y^3, n\ge 2\end{cases}$$

Alternate chain of Pentagons [ACP] :

An alternate chaining of pentagons ACP(n) is a graph consisting to n pentagonal rings, every two successive rings have a common edge, forming a chain as

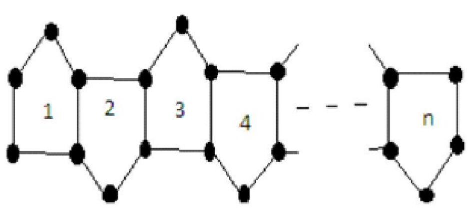

Figure 2 ACP, when n is even

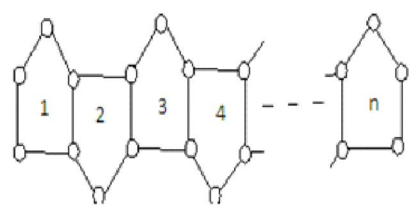

Figure 3 ACP, when n is odd

The number of edges are calculated for the various combinations of i,j and also for the number of pentagons n=2,4,6 from the graph of ACP in figure 2 and the results are tabulated below:

i,j	n=2	n=4	n=6
2,2	4	4	4
2,3	4	8	12
3,3	1	5	9

If ACP(n) is an alternate chain of pentagons, $n \geq 2$, n represents the number of pentagons, when n is even in ACP(n), then

$$M(ACP(n); x, y) = \{4x^2y^2 + 2n\,x^2y^3 + (2n-3)x^3y^3, n \geq 2 \textit{ also n is even}$$

The number of edges are calculated for the various combinations of i,j and also for the number of pentagons n=1,3,5,7 from the graph of ACP in figure 3 and the results are tabulated below:

i,j	n=1	n=3	n=5	n=7
2,2	5	4	4	4
2,3	5	6	10	14
3,3	5	3	7	11

If G(n) is an alternate chain of pentagons, $n \geq 2$, n represents the number of pentagons and n is odd in G(n), then

$$M(G(n); x, y) = \begin{cases} 5x^2y^2, n = 1 \\ 4x^2y^2 + 2n\,x^2y^3 + (2n-3)x^3y^3, n \geq 3(\textit{ for odd}) \end{cases}$$

Double row Penta-chains [DPCI] :

The graphs consisting of two rows of straight chains with n 5-cycles in the two rows combined. There are two types of double row penta chains.

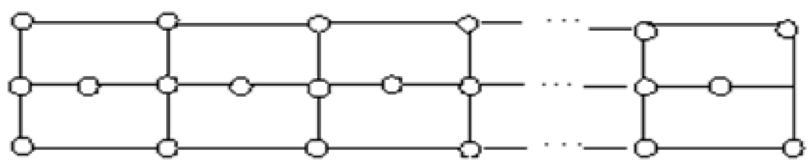

Figure 4 DPCI (Type I)

The number of edges are calculated for the various combinations of i,j and also for the number of pentagons n=2,4,6,8 from the graph of DPCI in figure 4 and the results are tabulated below:

i,j	n=2	n=4	n=6	n=8
2,2	0	0	0	0
2,3	10	10	10	10
2,4	0	2	10	14
3,4	4	6	10	14
3,3	0	4	8	12

If DPCI(n) is double row penta-chain of type I, $n \geq 2$, n represents the number of pentagons and n is even in DPCI(n), then

$$M(DPCI(n); x, y) = \begin{cases} 10\,x^2y^3 + 4x^3y^4, n = 2 \\ 10\,x^2y^3 + (2n-2)x^2y^4 + (2n-4)x^3y^3 \\ \qquad + (2n-2)x^3y^4, n > 2 \textit{ and also n is even} \end{cases}$$

The number of edges are calculated for the various combinations of i,j and also for the number of pentagons n=1,3,5,7 from the graph of DPCI in figure 4 and the results are tabulated below:

i,j	n=1	n=3	n=5	n=7
2,2	2	0	0	0
1,3	2	2	2	2
2,3	4	8	8	8
3,3	0	2	6	10
1,4	0	4	8	12

If DPCI(n) is double row penta chain of type I, $n \geq 2$, n represents the number of pentagons and n is odd in DPCI(n), then

$$M(DPCI(n);\ x, y) = \begin{cases} 2\,x^1y^3 + 2x^2y^2 + 4x^2y^3, n = 1 \\ 2x^1y^3 + 8x^2y^3 + (2n-2)x^1y^4 \\ \qquad + (2n-4)x^3y^3, n > 2 \textit{ and also n is odd} \end{cases}$$

Double row Penta-chains [DPCII] :

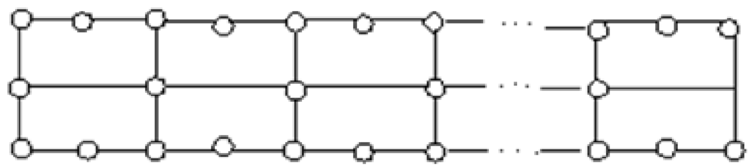

Figure 5 DPCII (Type II)

The number of edges are calculated for the various combinations of i,j and also for the number of pentagons n=2,4,6,8 from the graph of DPCII in figure 5 and the results are tabulated below:

i,j	n=2	n=4	n=6	n=8
2,2	0	4	4	4
2,3	12	16	24	24
3,4	4	8	12	16
4,4	0	2	4	6

If DPCII(n) is double row penta chain of type II, $n \geq 2$, n represents the number of pentagons and n is even in DPCII(n), then

$$M(DPCII(n); x, y) = \begin{cases} 12\,x^2y^3 + 4x^3y^4, n = 2 \\ 4n\,x^2y^3 + 4x^2y^2 + 2nx^3y^4 \\ \qquad + (n-2)x^4y^4, n \geq 4 \textit{ and also n is even} \end{cases}$$

The number of edges are calculated for the various combinations of i,j and also for the number of pentagons n=1,3,5,7 from the graph of DPCII in figure 5 and the results are tabulated below:

i,j	n=1	n=3	n=5	n=7
2,2	4	4	4	4
2,3	4	12	20	28
3,3	1	0	0	0
3,4	0	6	10	14
4,4	0	1	3	5

If G(n) is double row penta-chain of type II, $n \geq 2$, n represents the number of pentagons and n is odd in G(n), then

$$M(G(n); x, y) = \begin{cases} 4x^2y^2 + 4x^2y^3 + x^3y^3, n = 1 \\ 4x^2y^2 + 4nx^2y^3 + 2nx^3y^4 \\ \qquad + (n-2)x^4y^4, n \geq 3 \textit{ and also n is odd} \end{cases}$$

Conclusion

The vertex degree based topological indices are calculated for Straight Chaining of Pentagons, Alternate Chaining of Pentagons, Double Chaining of Pentagons of two types I and II. Topological index values calculated by using M-Polynomial are accurate and it can be calculated for higher powers of n for both odd and even. This polynomials are very helpful for the chemists to find the indices values for the molecular graphs algorithmically.

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