

TOPOLOGICAL INDEX OF VPH [m,n] NANOTORUS

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The Szeged index is one of the topological index defined in mathematical-chemistry. In this paper, Szeged index of v-phenylenic(VPH[m,n]) nanotorus, is computed for the first time.

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1.Introduction

Suppose that G be molecular graph the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. A topological index of a graph G is a numeric quantity related to G . The oldest topological index is the Wiener index. Numerous of its chemical applications were reported and its mathematical properties are well understood.¹⁻⁴

In Refs [5-9] the authors defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI. This newly proposed topological index does not coincide with the Wiener index for acyclic molecules.

The Szeged index is another topological index which is introduced by Ivan Gutman.¹⁰⁻¹³ To define the Szeged index of a graph G , we assume that $e = uv$ is an edge connecting the vertices u and v . Suppose $N_u(e|G)$ is the number of vertices of G lying closer to u and $N_v(e|G)$ is the number of vertices of G lying closer to v . Edges equidistance from u and v are not taken into account. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv \in E(G)} N_u(e|G)N_v(e|G)$, see also Ref [14].

In Refs. [15-20] the PI and Szeged indices of some hexagonal graphs containing nanotubes and nanotorus are computed. In this paper, we continue this work to compute the Szeged index of V- phenylenic VPH[m,n] nanotorous . Our notation is standard and mainly taken from Refs [21, 22].

2.Results and discussion

Phenylenic nanotorus are molecular graphs such that covered by C_6 , C_4 and C_8 . In this section, the szeged index of a V-Phenylenic VPH[m,n] nanotorus is computed. Following Diudea [23] we denote a V-Phenylenic nanotorus by $H=VPH [m,n]$.

In the following theorem we compute the szeged index of the molecular graph H in Fig. 1.

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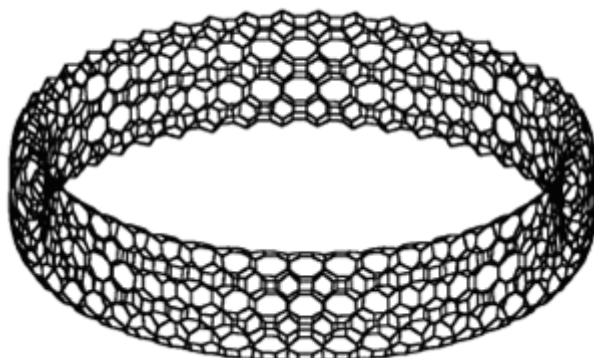


Fig. 1 . Phenylene nanotorus ;VPH[12,144]

Theorem 1. $Sz(H)=\begin{cases} X & \text{if } m < n \\ Y & \text{if } m = n \\ Z & \text{if } m > n \end{cases}$; where

$$X=168m^3n-24m^2n+528m^5+84m^3-12m^2-936m^4n-24m^4+216m^3n^3+120m^3n-12mn^3+648m^5n-720m^4n^2+576m^3n^2-72m^2n^3+144m^3n-144m^2n^2-168m^6+72m^3n^2+96m^2n^3-24m^4+24mn^3+36mn^2+12mn,$$

$$Y =4n(6mn-3(n+1)^2)(-6+3(n+1)^2)+48m^3n^3-24m^3n-6n^3m \text{ and}$$

$$Z=300mn^3-24mn^2-24n^5+12nm-504mn^4+312m^3n^3+360m^2n^3-288m^2n^4+144mn^4-72m^3n^2+72n^5m+24n^6+72n^5-36n^4-12n^3-24n^4+36nm^2.$$

Proof. To prove, assume that A_1, A_2 and A_3 to be the set of all vertical, oblique and horizontal edges, respectively.

if $e_i = u_i v_i$ be an edge in A_i ($i=1,2$) on j^{th} rows , then the results in table1 are obtained.

Table 1 . $N_{u_i}(e_i)$ and $N_{v_i}(e_i)$ for vertical and horizontal edges

Edge	$N_{u_i}(e_i)$	$N_{v_i}(e_i)$
e_1	$6mj$	$(6mn-6mj)(2m)$
e_2	$3nj$	$(6mn-3mj)(2n)$

And finally if $e_3 = u_3 v_3$ be an oblique edge of A_3 , then these following two cases in table 2 are arisen :

Table 2 . $N_{u_i}(e_i)$ and $N_{v_i}(e_i)$ for an oblique edge.

cases	$N_{u_3}(e_3)$	$N_{v_3}(e_3)$
$m \neq n$	$2\beta(S\beta+(6\beta-3)j)$	$6mn- S\beta-(6\beta-3)j$
$m=n$	$4n(S_n+6n-3)$	$(6nm- S_n-6n+3)$

Where $S_k = 3+9+15+\dots + (6k-3)$ and $\beta = \min(m,n)$.

By above tables and definition of szeged index , proof is completed. ■

3. Conclusion

A topological index is any of several numerical parameters of molecular graph G which characterize its topology. It is a kind of a molecular descriptor. In this paper, most important topological index called "szeged index" of $VPH[m,n]$ nanotorus, is computed.

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References

- [1] H. Wiener, *J. Am. Chem. Soc.* **69**, 17(1947).
- [2] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley, Weinheim, 2000.
- [3] D.E. Needham, I.C. Wei, P.G. Seybold, *J. Am. Chem. Soc.* **110**, 4186(1988).
- [4] G. Rucker, C. Rucker, *J. Chem. Inf. Comput. Sci.* **39**, 788(1999).
- [5] P. V. Khadikar, *Nat. Acad. Sci. Lett.* **23**, 113(2000).
- [6] P. V. Khadikar; P.P. Kale; N.V. Deshpande; S. Karmarkar, V.K. Agrawal, *J. Math. Chem.* **29**, 143(2001).
- [7] P.V. Khadikar; S. Karmarkar, *J. Chem. Inf. Comput. Sci.* **41**, 934(2001).
- [8] P.V. Khadikar, S. Karmarkar, R.G. Varma, *Acta Chim. Slov.* **49**, 755(2002).
- [9] M. V. Diudea, M. S. Florescu, P. V. Khadikar, *MATCHCommun. Math. Comput. Chem* **58**, 233(2007).
- [10] I. Gutman, *Graph Theory Notes of New York* **27**, 9(1994).
- [11] A. Das, G. Domotor, I. Gutman, S. Joshi, S. Karmarkar, D. Khaddar, T. Khaddar, P. V. Khadikar, L. Popovic, N.S. Sapre, N. Sapre, A. Shirhatti, *J. Serb. Chem. Soc.* **62**, 235(1997).
- [12] O. M. Minailiuc, G. Katona, M. V. Diudea, M. Strunje, A. Graovac, I. Gutman, *Croat. Chem. Acta* **71**, 473(1998).
- [13] M. V. Diudea, I. Gutman, *Croat. Chem. Acta*, **71**, 21(1998).
- [14] S. Karmarkar, S. Karmarkar, S. JOSHI, A. DAS, P. V. Khadikar, *J. Serb. Chem. Soc.* **62**, 227(1997).
- [15] A.R.Ashrafi and A.Loghman, *J. Comput. Theor. Nanosci.* **3**, 378(2006).
- [16] S.Yousefi and A.R.Ashrafi, *MATCHCommun. Math. Comput.Chem.* **55**, 169(2006).
- [17] A.R.Ashrafi and F.Rezaei, *MATCHCommun. Math. Comput.Chem.* **57**, 243 (2007).
- [18] A.R.Ashrafi and A.Loghman, *J. Chil. Chem. Soc.* **51**, 968 (2006).
- [19] H. Yousefi, A.R. Ashrafi, A. Bahrami, *J. Comput. Theor. Nanosci.* **4**, 1(2007).
- [20] A.Bahrami, J.Yazdani, *Digest Journal of Nanomaterials and biostructures.* **4**, 265 (2008).
- [21] P.J. Cameron, *Combinatorics: Topics, Techniques, Algorithms*, Cambridge University Press, Cambridge, 1994.
- [22] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL. 1992.
- [23] M.V.Diudea, *Fuller. Nanotub. Carbon Nanostruct.* **10**, 273 (2002).