Some conjectures on energy and Estrada index of *$CNC_k[n]$*nanocones

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In this paper, we suggest conjectures to approximate the values of energy and Estrada index of *$CNC_k[n]$* nanocones using computational tools. We conjecture that the energy and Estrada index of *$CNC_k[n]$* nanocones, $k \geq 3$, can be estimated by the curves$(2.56(k-2)+5.12)n^{1.854}+3.87(k-2)+7.717$ and $(5.21(k-2)+10.41)n^{1.861}+4.585(k-2)^{1.225}+18.85$, respectively.

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1. Introduction

Carbon nanocones have been observed since 1968 or even earlier [10], on the surface of naturally occurring graphite. Their bases are attached to the graphite and their height varies between 1 and 40 micrometers. Their walls are often curved and are less regular than those of the laboratory made nanocones.

Carbon nanostructures have attracted considerable attention due to their potential use in many applications including energy storage, gas sensors, biosensors, nanoelectronic devices and chemical probes [15]. Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices [1, 20]. More recently, carbon nanocones have gained increased scientific interest due to their unique properties and promising uses in many novel applications such as energy and gas storage [19].

Let G be an n-vertex molecular graph with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge set $E(G)$. The vertices of G correspond to atoms and an edge between two vertices corresponds to the chemical bond between these vertices. The *adjacency matrix* $A(G)=[a_{ij}]_{n\times n}$ of the graph G is defined by:

$$a_{ij}=\begin{cases}1 & v_iv_j \in E(G)\\ 0 & otherwise\end{cases}(\forall\, v_i,v_j \in V(G)).$$

The *characteristic polynomial* of G is denoted by $\Phi(G,\lambda)$ and is defined by

$$\Phi(G,\lambda)=\det(\lambda I_n - A(G)),$$

where I_n denotes the identity matrix of order n. The roots of $\Phi(G,\lambda)=0$ are called the eigenvalues of G; we denote these eigenvalues by $\lambda_1,\lambda_2,\ldots,\lambda_n$. The multiset of eigenvalues of *G* is called the *spectrum* of *G*. Since a molecular graph G is simple, the matrix $A(G)$ is real and symmetric with zero trace. Thus all eigenvalues of G are real and their sum is zero [4]. The *energy* of the graph G is defined by

$$E(G)=\sum_{i=1}^{n}|\lambda_i|. \tag{1}$$

This mathematical quantity was first proposed by Gutman [12] in 1978. However, its chemical roots lie in Hückel Molecular Orbital Theory, which was proposed in 1930's. Hückel's method allows a chemist to approximate the energies associated to the π-electron orbitals in conjugated hydrocarbons. This graph invariant correlates well with the chemical quantity known as total π-electron energy of conjugated hydrocarbon molecules [14]. For more details of graph energy and its chemical significance, see [4, 11, 13, 19].

Estrada [5] introduced a graph-spectrum based invariant; called the *Estrada index* and defined it by

$$EE(G)=\sum_{i=1}^{n}\exp^{\lambda_i}. \tag{2}$$

Since its invention, the Estrada index has found noteworthy chemical applications. It is used to quantify the degree of folding of proteins and some other long-chain biomolecules [5, 6, 7]. Moreover, Estrada and RodrAguez [9] have shown that the Estrada index provides a measure of centrality of complex networks. Recently, Ashrafi et al. [2, 3] and Malik et al. [16] studied the energy and Estrada index of nanotubes and nanocones. For further details, the reader is referred to [8, 17].

The molecular graph of $CNC_k[n]$ nanocones has a conical structure with a cycle of length k at its core and n layers of hexagons placed at the conical surface around its center (see Fig. 1). Ashrafi and Sadati [3] suggested a curve to estimate the energy and Estrada index of $CNC_5[n]$ nanocones. In this paper, we estimate the energy and Estrada index of $CNC_k[n]$ nanocones for $k \geq 3$ by suggesting general curves. These curves give much better approximations of energy and Estrada index of $CNC_5[n]$ as compared to the curves suggested by Ashrafi and Sadati [3].

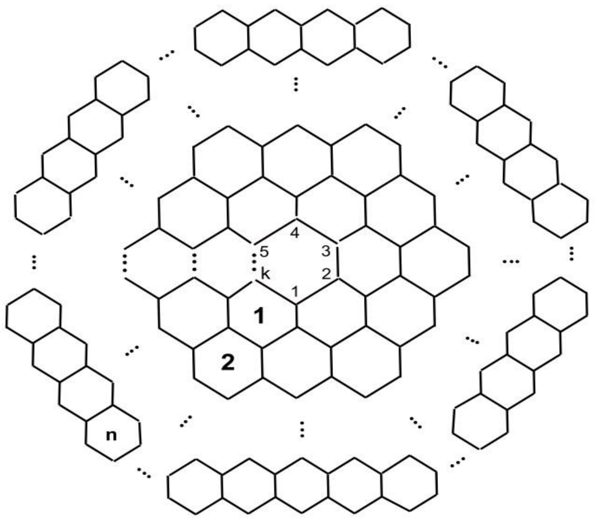

Fig. 1. The graph of $CNC_k[n]$ nanocone.

2. Energy and Estrada index of $CNC_k[n]$ nanocones (for $k=3,4,5$)

In this section, we explain the computational procedure to calculate the energy and Estrada index of $CNC_k[n]$ nanocones for $k = 3,4,5$.

The molecules of $CNC_3[n]$ are drawn in HyperChem [21] for $1 \leq n \leq 11$. The adjacency matrices of these molecular graphs are constructed with the help of TopoCluj [18]. Then the energy and Estrada index are calculated using MATLAB. The obtained data is shown in Table 1.

By using "cftoolbox" of MATLAB, a power curve of the form $an^b + c$ is fitted to the data shown in Table 1. A polynomial can approximate a smooth curve with small error and the curves with exponential increase are better fitted with power or exponential functions. Our calculations show that the behaviour of energy and Estrada index of nanocones is exponential. Thus the energy and Estrada index of $CNC_3[n]$ nanocones can be estimated by the following curves:

$$E(CNC_3[n]) \cong 7.68n^{1.854} + 11.75, \quad (3)$$

$$EE(CNC_3[n]) \cong 15.62n^{1.861} + 23.44. \quad (4)$$

Next, we calculate $E(CNC_4[n])$ and $EE(CNC_4[n])$ by following the same procedure as we followed before. The curves given by equations (5) and (6), estimating the energy and Estrada index of $CNC_4[n]$, are obtained from the data presented in Table 2.

$$E(CNC_4[n]) \cong 10.24n^{1.854} + 15.13, \quad (5)$$

$$EE(CNC_4[n]) \cong 20.83n^{1.861} + 29.57. \quad (6)$$

Table 1. The exact values of energy and Estrada index of $CNC_3[n]$ nanocones, $1 \leq n \leq 11$, calculated by using equations (1) and (2).

n	Energy	Estrada index
1	17.2859184602652	34.90228208693608
2	39.92799424358724	80.96364519114939
3	71.95828121952398	146.6524905652332
4	113.3970122940882	231.9695783788370
5	164.2574898928459	336.9149088724020
6	224.5486057576022	461.4884820459496
7	294.2762041727111	605.6902978994802
8	373.4440212903026	769.5203564329929
9	462.0544073288664	952.9786576464878
10	560.1088533736765	1156.065201539966
11	667.6083318445358	1378.779988113426

Table 2. The exact values of energy and Estrada index of $CNC_4[n]$ nanocones, $1 \leq n \leq 11$, calculated by using equations (1) and (2).

n	Energy	Estrada index
1	22.6552379446429	44.8518750239294
2	52.4773417297321	106.266119700321
3	95.4991278556304	193.851246567694
4	150.572271474423	307.607363652473
5	218.542216587352	447.534470977226
6	298.839920372652	613.632568541957
7	391.886727620073	805.901656346664
8	497.402271470619	1024.34173439135
9	615.582318258625	1268.95280267601
10	746.305658242764	1539.73486120065
11	889.649819060568	1836.68790996526

Ashrafi and Sadati [3] conjectured that the energy and Estrada index of $CNC_5[n]$ nanocones can be estimated by the equations

$$E(CNC_5[n]) = 28.7372(1.2)^{n-1}, \quad (7)$$

$$EE(CNC_5[n]) = 55.5639(1.2)^{n-1}. \quad (8)$$

The exact values of energy and Estrada index of

CNC_5[n] nanocones calculated by using equations (1) and (2) are given in Table 3. Our calculations suggest that the energy and Estrada index of *CNC_5[n]* nanocones can be estimated by the exponential curves given by

$$E(CNC_5[n]) \cong 12.8n^{1.854} + 19.49, \qquad (9)$$

$$EE(CNC_5[n]) \cong 26.04n^{1.861} + 36.46. \qquad (10)$$

One can easily check that the equations (9) and (10) give higher accuracy as compared to equations (7) and (8). For example, for $n = 11$ the equations (7) and (8) give

$$E(CNC_5[11]) = 177.93317, \quad EE(CNC_5[11]) = 344.03702.$$

However, equations (9) and (10) give

$$E(CNC_5[11]) = 1110.8097, \quad EE(CNC_5[11]) = 2294.1939,$$

which is much closer to the exact values of energy and Estrada index of *CNC_5[n]* nanocones.

Table 3. The exact values of energy and Estrada index of CNC_5[n] nanocones, $1 \le n \le 11$, calculated by using equations (1) and (2).

n	Energy	Estrada index
1	28.73724086797208	55.56392932367799
2	66.43060911255543	132.3316121087914
3	119.8435927566387	241.8130206666559
4	188.8925953205016	384.0081670226269
5	273.6709036427948	558.9170511785687
6	374.1500925987631	766.5396731344816
7	490.3666383558780	1006.876032890366
8	622.3109849474412	1279.926130446221
9	769.995980912568	1585.68996580205
10	933.4195515448562	1924.167538957842
11	1112.585456091773	2295.358849913610

3. Energy and Estrada index of *CNC_k[n]* nanocones (for $k \ge 3$)

One can observe that the equations (3), (5) and (9) are of the form $an^b + c$. Here $b = 1.854$ and the coefficients a and c increase linearly. We estimate the coefficients a and c, for $k \ge 3$, as follows

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$$a = 2.56(k-2) + 5.12, \quad c = 3.87(k-2) + 7.717.$$

Similarly, the equations (4), (6) and (10), are of the form $an^b + c$. Here $b = 1.861$ and the coefficients a and c respectively increase linearly and exponentially. We estimate the coefficients a and c, for $k \ge 3$, as follows.

$$a = 5.21(k-2) + 10.41, \quad c = 4.585(k-2)^{1.225} + 18.85.$$

We suggest general curves to estimate the energy and Estrada index of *CNC_k[n]* nanocones ($k \ge 3$ and $n \ge 1$) by

$$E(CNC_k[n]) = (2.56(k-2) + 5.12)n^{1.854} + 3.87(k-2) + 7.717, \qquad (11)$$

$$EE(CNC_k[n]) = (5.21(k-2) + 10.41)n^{1.861} + 4.585(k-2)^{1.225} + 18.85. \qquad (12)$$

4. Analysis of the results and conclusion

Since the molecular graphs have usually large order, it becomes very hard to obtain and handle their data. In such cases, the computational and statistical methods provide very useful tools. These tools reduce the time and effort that is required to perform a certain task. In this context, we have estimation tools to obtain the desired quantities by extrapolation. We have derived the approximation curves given by equations (11) and (12) for the energy and Estrada index of *CNC_k[n]* nanocones. Some estimated values of $E(CNC_k[n])$ and $EE(CNC_k[n])$ calculated from equations (11) and (12), respectively, are compared with the corresponding exact values in Table 4.

For $k \in \{3,4,\ldots,10\}$ the curves given by equations (11) and (12) give a good approximation of energy and Estrada index of *CNC_k[n]* nanocones. However, it is not certain that (11) and (12) can give a good approximation of energy and Estrada index for larger values of k .

Table 4. Comparison of exact values of energy and Estrada index of $CNC_k[n]$ nanocones calculated by using equations (1) and (2) with the corresponding estimated values calculated by using (11) and (12).

$[k,n]$		Energy	Estrada index
[5,12]	Exact	1307.493926	2699.263899
	Estimated	1301.693015	2691.051099
[5,13]	Exact	1518.146055	3135.882685
	Estimated	1506.840599	3117.446990
[7,4]	Exact	264.4223902	537.4529550
	Estimated	261.2510052	532.8954912
[7,5]	Exact	383.1230028	782.325393
	Estimated	381.2505556	780.5646281
[8,4]	Exact	302.0061802	614.2283756
	Estimated	298.5758631	609.8857596
[8,5]	Exact	437.7879216	894.0825902
	Estimated	435.7182063	892.9459060
[9,5]	Exact	492.5828863	1005.842418
	Estimated	490.1858572	1005.643401
[9,6]	Exact	673.4318294	1379.563137
	Estimated	673.3275706	1384.185845
[10,5]	Exact	547.3418073	1117.602626
	Estimated	544.6535079	1118.621264

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