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Energy and Laplacian Energy-Like Invariant of Unicyclic Molecular Graphs

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ABSTRACT

Let Un be the set of unicyclic molecular graphs with $3 \leq n \leq 8$ vertices. We show that the cycle Cn has maximal Laplacian-energy-like invariant (LEL) in Un. The authors partially proving that the conjecture hold for any unicyclic molecular graph in Un, where $3 \leq n \leq 8$ Moreover, we show that Cn has maximal energy (E) in Un for $3 \leq n \leq 7$, but for n=8 this is not true.

Keywords: Molecular graphs, Laplacian energy-like invariant, Energy

INTRODUCTION

The total π-electron energy E, as calculated within the Huckel molecular orbital (HMO) model, is one of the most thoroughly studied quantum-chemical characteristics of large polycyclic conjugated molecules. Details on the theory and applications of E can be found in the literature [1-3] and in the references cited therein. It was recognized a long time ago that the various π-electron descriptors of HMO model, including E, can be calculated from the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda n$ of the underline molecular graph [4,5]. In particular, in the case of alternant hydrocarbons.

$$E = \sum_{i=1}^{n} |\lambda_i| \qquad (1)$$

Where, as usual [1,2,4,5] E is expressed in the units of the HMO carbon-carbon resonance integral β. Formula (1) served as a motivation for the definition of the so-called graph energy. Namely, whereas within the HMO model E is meaningful only in the case of a restricted class of molecular graphs [5], the right-hand side of (1.1) is a well-defined quantity for all graphs. In view of this, the energy of a graph (also denoted by E) is defined as the sum of the absolute values of all eigenvalues of this graph, and this definition extends to all graphs. This seemingly insignificant change in the interpretation of Equation. (1) resulted in a great expansion of research in this area and has advanced the theory of total π-electron energy greatly; for details see the reviews [1,6] and some of the most recent publications dealing with graph energy [7-13].

By equation (1), the graph energy is defined in terms of the graph eigenvalues λ_1, λ_2

,..., λn. Recall that these are just the eigenvalues of the adjacency matrix [14]. Motivated by the success of the graph energy concept, and in order to extend it to the Laplacian eigenvalues, the Laplacian energy LE(G) was put forward, defined as

$$LE = LE(G) = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n}| \qquad (2)$$

Where *G* is a graph with *n* vertices and *m* edges, and $\mu_1, \mu_2, \ldots, \mu_n$ are its Laplacian eigenvalues [15]. The Laplacian energy has two major drawbacks: Namely, neither $LE(G_1 \cup G_2)=LE(G_1)+LE(G_2)$ holds in the general case, for $G_1 \cup G_2$ being the graph consisting of two disconnected components G_1 and G_2, nor is the condition $LE(G \cup K_1)=LE(G)$, where K_1 is the graph with single vertex, satisfied. In order to overcome these difficulties, Liu and Liu invented the *Laplacian energy-like invariant LEL* (*G*), defined as [16].

$$LEL = LEL(G) = \sum_{i=1}^{n} \sqrt{\mu_i} \tag{3}$$

Indeed, the relations LEL (G_1 [G_2)=LEL(G_1) + LEL (G_2) and LE(G] K_1)=LE(G) are generally vaild.

The theory of LEL is nowadays well developed; details and further references can be found in the review [17]. In particular, numerous correlations between LEL and physico-chemical properties of alkanes were reported [18]. It was shown that, in spite of its name, LEL resembles more the total π-electron energy than the Laplacian energy LE [19]. It is known that the main parameters determining the value of the total π-electron energy are n (= the number of carbon atoms, i.e, the number of vertices of the molecular graph) and m (= the number of carbon- carbon bonds, i.e, the number of edges of the molecular graph) [1,20].

In [21], Stevanovi´c studied the LEL of trees (trees are connected acyclic graphs). In that paper he conjectured the following conjecture as well

Conjecture 1.1 Among unicyclic molecular graphs on n vertices, the cycle Cn has maximal Laplacian energy-like invariant.

The main purpose of the present paper is to give the partial proof of the conjecture (1.1). That is we will prove that the conjecture 1.1 is true for $3 \le n \le 8$. Moreover, we will show that among molecular unicyclic graphs the cycle Cn has maximal energy E for $3 \le n \le 7$ but for n=8 it is not true. Where n is the number of vertices in the unicyclic molecular graph.

For unexplained terminology see the following subsection

Definitions: Let G=(V, E) be a simple connected molecular graph with vertex set V={v_1, v_2,..., vn} and edge set E={e_1, e_2,..., en}. Its adjacency matrix A(G)=(aij) is defined as n × n matrix (aij), where aij=1 if vi is adjacent to vj; and aij=0, otherwise. Denote by d(vi) or dG(vi) the degree of the vertex vi (number of adjacent vertices to vi). The matrix L(G)=D(G) − A(G) is called the Laplacian matrix of graph G, where D(G)=diag(d_{v1}, d_{v2},..., d_{vn}) denotes the diagonal matrix of vertex degrees of G.

Definition: A unicyclic molecular graph is a connected graph G containing exactly one cycle.

UNICYCLIC MOLECULAR GRAPHS

In this section, we will give all unicyclic molecular graphs with at most 8 vertices.

Lemma

There are exactly 143 unicyclic molecular graphs with $3 \le n \le 8$ vertices.

Proof. From [22, p. 213-215] one can find all unicyclic molecular graphs for $3 \le n \le 8$, where n is the number of vertices in the unicyclic molecular graph G

On (**Figure 1)**, we give all the diagrams of the 54 unicyclic molecular graphs with at most 7 vertices. On (**Figure 2)**, we give all the diagrams of the 89 unicyclic molecular graphs with exactly 8 vertices. We denote all these unicyclic molecular graphs by Ui for i=1,..., 143. Clearly, on (**Figure 1)**, U_1 is a cycle C_3, U_3 is a cycle C_4, U_8 is a cycle C_5, $U_2$1 is a cycle C_6 and U_{54} is a cycle C_7. On **Figure 2**, U_{143} is a cycle C_8.

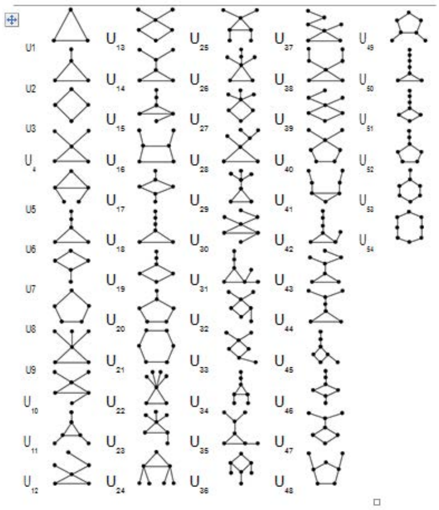

Figure 1: Diagrams of the 54 unicyclic molecular graphs with at most 7 vertices.

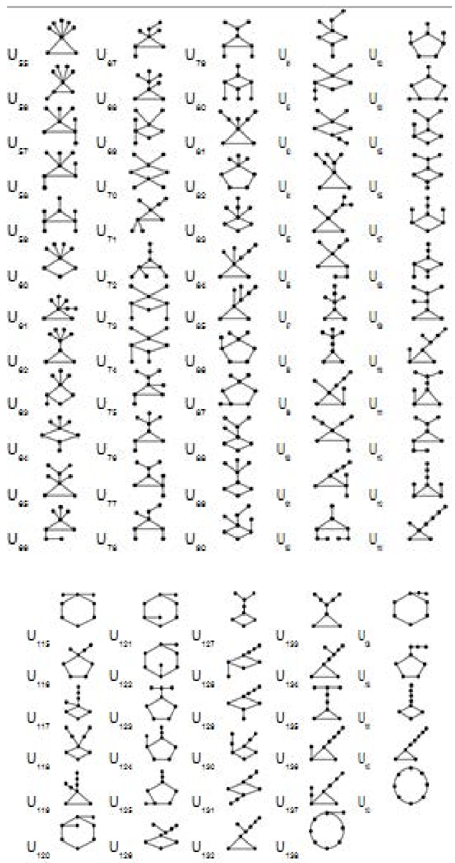

Figure 2: Diagrams of the 89 unicyclic molecular graphs with exactly 8 vertices.

PARTIAL PROOF OF THE CONJECTURE

From, (**Figure 1 and 2)**, we have all unicyclic molecular graphs Ui for i=1,..., 143 with at most 8 vertices. In the first column of the following tables (Tables 1-3), we give the name Ui for i=1,..., 143, in the second column the number of vertices n, in the third column the Laplacian spectrum and in the fourth column we give Laplacian energy-like invariant LEL. By direct calculation (one can do this exercise by computer, by use of suitable mathematical softwares, for example Matlab or athematica) we find the Laplacian spectrum of each unicyclic molecular graph Ui and the Laplacian energy-like invariant LEL.

Now, if n=3, then we have only one unicyclic molecular graph $U_1=C_3$, with LEL ≈ 3.4146, for n=4, $U_3=C_4$ has the maximal LEL among all unicyclic molecular graphs with 4 **(Tables 1 and 2)** vertices, for n=5, $U_8=C_5$ has the maximal LEL among all unicyclic molecular graphs with 5 **(Table 3)** vertices, for n=6, $U_{21=}C_6$ has the maximal LEL among all the unicyclic molecular graphs with 6 vertices, for n=7, $U_{54}=C_7$ has the maximal LEL among all unicyclic molecular graphs with 7 vertices and for n=8, $U_{143}=C_8$ has the maximal LEL among all unicyclic molecular graphs with 8 vertices. Consequently, we can see that the conjecture 1.1 is true for $3 \leq n \leq 8$.

Table 1: Partial proof of the conjecture.

#	n	Laplacian spectrum	LEL
U_1	3	0, 3, 3	3.4641
U_2	4	0, 1, 3, 4	4.7321
U_3	4	0, 2, 2, 4	4.8284
U_4	5	0, 0.5188, 2.3111, 3, 4.1701	6.0146
U_5	5	0, 0.6972, 1.3820, 3.6180, 4.3028	5.987
U_6	5	0, 1, 1, 3, 5	5.9681
U_7	5	0, 0.8299, 2, 2.6889, 4.4812	6.0819
U_8	5	0, 1.3820, 1.3820, 3.6180, 3.6180	6.1554
U_9	6	0, 0.3249, 1.4608, 3, 3, 4.2143	7.2956
U_{10}	6	0, 0.6571, 1, 2.5293, 3, 4.8136	7.327
U_{11}	6	0, 0.7639, 1, 2, 3, 5.2361	7.3085
U_{12}	6	0, 0.4384, 1, 3, 3, 4.5616	7.262
U_{13}	6	0, 0.4859, 1, 2.4280, 3, 5.0861	7.2426
U_{14}	6	0, 1, 1, 1, 1, 3, 6	7.1815
U_{15}	6	0, 0.6314, 1, 1.4738, 3.7877, 5.1071	7.2147
U_{16}	6	0, 0.4131, 1.1369, 2.3595, 3.6977, 4.3928	7.2639
U_{17}	6	0, 0.6972, 0.6972, 2, 4.3028, 4.3028	7.2328
U_{18}	6	0, 0.4384, 2, 2, 3, 4.5616	7.3584
U_{19}	6	0, 0.5858, 1.2679, 2, 3.4142, 4.7321	7.3287
U_{20}	6	0, 0.6972, 1.3820, 2, 3.6180, 4.3028	7.4012
U_{21}	6	0, 1, 1, 3, 3, 4	7.4641
U_{22}	7	0, 1, 1, 1, 1, 3, 7	8.3778
U_{23}	7	0, 0.5961, 1, 1, 1.5196, 3.8273, 6.0570	8.4222
U_{24}	7	0, 0.5505, 1, 1, 1.5858, 4.4142, 5.4495	8.4367
U_{25}	7	0, 0.6086, 0.6972, 1, 2.2271, 4.3028, 5.1642	8.4543
U_{26}	7	0, 0.4659, 1, 1, 2.4827,3, 6.0514	8.4502
U_{27}	7	0, 0.7269, 1, 1, 2, 3.1404, 6.1326	8.5153
U_{28}	7	0, 0.3983, 1, 1, 3, 3.3399, 5.2618	8.4846
U_{29}	7	0, 0.3983, 1, 1, 3, 3.3399, 5.2618	8.4846
U_{30}	7	0, 0.4116, 0.7530, 1.4064, 2.4450, 3.8019, 5.1819	8.4851
U_{31}	7	0, 0.3679, 1, 1.1879, 2.3732, 3.9464, 5.1228	8.4869
U_{32}	7	0, 0.5858, 1, 1, 2.5858, 3.4142, 5.4142	8.548
U_{33}	7	0, 0.5140, 1, 1.3364, 2, 3.8360, 5.3136	8.5514
U_{34}	7	0, 0.3820, 0.6972, 1.5858, 2.6180, 4.3028, 4.4142	8.5057
U_{35}	7	0, 0.3403, 1, 1.1451, 3, 3.8549, 4.6567	8.5075
U_{36}	7	0, 0.5858, 0.6837, 1.4206, 2.8654, 3.4142, 5.0303	8.5675
U_{37}	7	0, 0.2955, 1, 1.4911, 3, 3.1169, 5.09665	8.5198
U_{38}	7	0, 0.3820, 0.6086, 2.2271, 2.6180, 3, 5.1642	8.5131
U_{39}	7	0, 0.4330, 0.8510, 2, 2.3024, 3.1129, 5.3006	8.5787
U_{40}	7	0, 0.6086, 1, 1.3820, 2.2271, 3.6180, 5.1642	8.6227
U_{41}	7	0, 0.3004, 0.7530, 2.2391, 2.4450, 3.8019, 4.4605	8.5377
U_{42}	7	0, 0.2679, 1, 1.5858, 3, 3.7321, 4.4142	8.5418
U_{43}	7	0, 0.3217, 0.6802, 2.1397, 3, 3.2297, 4.6287	8.5353
$U_4$4	7	0, 0.2679, 1, 1.5858, 3, 3.7321, 4.4142	8.5418
U_{45}	7	0, 0.3820, 0.8851, 2, 2.6180, 3.2541, 4.8608	8.5997
U_{46}	7	0, 0.3588, 1, 2, 2.2763, 3.5892, 4.7757	8.6018

U_{47}	7	0, 0.3588, 1, 2, 2.2763, 3.5892, 4.7757	8.6018
U_{48}	7	0, 0.5188, 1, 1.5858, 2.3111, 4.1701, 4.4142	8.6429
		6	

Table 2 : Partial proof of the conjecture.

#	n	Laplacian spectrum	LEL
U_{49}	7	0, 0.6228, 0.7530, 1.7261, 2.4450, 3.8019, 4.6511	8.6409
U_{50}	7	0, 0.2254, 1, 2.1859, 3, 3.3604, 4.2283	8.5747
U_{51}	7	0, 0.2765, 1.3323, 2, 2.5219, 3.2920, 4.5772	8.6362
U_{52}	7	0, 0.3820, 1.3820, 1.5858 ,2.6180, 3.6180, 4.4142	8.6741
U_{53}	7	0, 0.5858, 1, 1.5858, 3, 3.4142, 4.4142	8.7055
U_{54}	7	0, 0.7530, 0.7530, 2.4450, 2.4450, 3.8019, 3.8019	8.7625
U_{55}	8	0, 1, 1, 1, 1, 1, 3, 8	9.5605
U_{56}	8	0, 1, 1, 1, 1.5468, 7.0362	9.6142
U_{57}	8	0, 0.5069, 1, 1, 1, 1.6400, 4.6654, 6.1877	9.6401
U_{58}	8	0, 0.5607, 0.9672, 1, 1, 2.3389, 4.3028, 6.1004	9.6573
U_{59}	8	0, 0.5505, 0.6571, 1, 1, 2.5293, 4.8136, 5.4495	9.9714
U_{60}	8	0, 0.7029, 1, 1, 1, 2, 3.2132, 7.0839	9.7067
U_{61}	8	0, 0.4592, 1, 1, 1, 2.5135, 3, 7.0340	9.6423
U_{62}	8	0, 0.3738, 1, 1, 1, 3, 3.4849, 6.1413	9.6884
U_{63}	8	0, 0.5449, 1, 1, 1, 2.5987, 3.6291, 6.2273	9.7507
U_{64}	8	0, 0.4746, 1, 1, 1.3691, 2, 4, 6.1563	9.7544
U_{65}	8	0, 0.3738, 1, 1, 1, 3, 3.4849, 6.1413	9.6884
U_{66}	8	0, 0.3417, 1, 1, 1.2176, 2.3795, 4, 6.0612	9.6925
U_{67}	8	0, 0.4103, 0.6758, 1, 1.4853, 2.4907, 3.8322, 6.1057	9.6881
U_{68}	8	0, 0.3542, 1, 1, 1, 3, 4, 5.6458	9.7033
U_{69}	8	0, 0.5107, 1, 1, 1, 2.7108, 4, 5.7785	9.7649
U_{70}	8	0, 0.4384, 1, 1, 1.4384, 2, 4.5616, 5.5616	9.7698
U_{71}	8	0, 0.3676, 0.7223, 1, 1.5047, 2.4500, 4.4669, 5.4885	9.7044
U_{72}	8	0, 0.3568, 0.6365, 1, 1.6887, 2.7571, 4.3873, 5.1735	9.7242
U_{73}	8	0, 0.5858, 0.5858, 1, 1.4384, 3.4142, 3.4142, 5.5616	9.7839
U_{74}	8	0, 0.5066, 0.6743, 1, 1.4986, 2.8999, 3.9168, 5.5038	9.7851
U_{75}	8	0, 0.3339, 0.7460, 1, 1.4123, 3.3136, 3.8587, 5.3356	9.7245
U_{76}	8	0, 0.3030, 1, 1, 1.1479, 3.2427, 4, 5.2863	9.7218
U_{77}	8	0, 0.2967, 1, 1, 1.2048, 3, 4.3310, 5.1675	9.7287
$U_7$8	8	0, 0.3820, 0.6972, 0.7639, 2, 2.6180, 4.3028, 5.2361	9.7219
U_{79}	8	0, 0.3065, 0.6972, 1, 1.6703, 3.3297, 4.3028, 4.6935	9.7465
U_{80}	8	0, 0.5858, 0.5858, 0.7639, 2, 3.4142, 3.4142, 5.2361	9.8027
U_{81}	8	0, 0.3820, 0.5607, 1, 2.3389, 2.6180, 3, 6.1004	9.7162
U_{82}	8	0, 0.5607, 1, 1, 1.3820, 2.3389, 3.6180, 6.1004	9.8257
U_{83}	8	0, 0.4284, 0.7828, 1, 2, 2.4204, 3.1905, 6.1779	9.781
U_{84}	8	0, 0.2774, 1, 1, 1.5068, 3, 3.1610, 6.0548	9.7248
U_{85}	8	0, 0.2888, 0.6742, 1, 2.1694, 3, 3.5857, 5.2819	9.7553
U_{86}	8	0, 0.5447, 0.7347, 1, 1.7635, 2.7242, 3.9063, 5.3266	9.858
U_{87}	8	0, 0.4484, 1, 1, 1.6280, 2.4815, 4.2659, 5.1762	9.8614
U_{88}	8	0, 0.3479, 0.8495, 1, 2, 2.7627, 3.6076, 5.4323	9.818
U_{89}	8	0, 0.3187, 1, 1, 2, 2.3579, 4, 5.3234	9.8215
U_{90}	8	0, 0.3820, 0.7254, 1, 2.3000, 2.6180, 3.5096, 5.4651	8.5418
U_{91}	8	0, 0.3581, 0.6918, 1.2843, 2, 2.4091, 3.8877, 5.3689	9.8186
U_{91}	8	0, 0.3479, 0.8495, 1, 2, 2.7627, 3.6076, 5.4323	9.818
U_{93}	8	0, 0.3187, 1, 1, 2, 2.3579, 4, 5.3234	9.8215
U_{94}	8	0, 0.3187, 0.5858, 1, 2.3579, 3, 3.4142, 5.3234	9.7525
U_{95}	8	0, 0.2384, 1, 1, 1.6367, 3, 4, 5.1249	9.7635
U_{96}	8	0, 0.2955, 0.5979, 1449, 2.3295, 2.4734, 3.9635, 5.1952	9.756
		7	

Table 3 : Partial proof of the conjecture.

#	n	Laplacian spectrum		LEL
U_{97}	8	0, 0.3187, 0.5858, 1, 2.3579, 3, 3.4142, 5.3234		9.7525
U_{98}	8	0, 0.2384, 1, 1, 1.6367, 3, 4, 5.1249		9.7635
U_{99}	8	0, 0.2593, 0.7150, 1.3232, 1.5891, 3.1143, 3.8086, 5.1905		9.7603
U_{100}	8	0, 0.3820, 0.4280, 1.2285 ,2.2799, 2.6180, 3.8123, 5.2513		9.7527
U_{101}	8	0, 0.2384, 1, 1, 1.6367, 3, 4, 5.1249		9.7635
U_{102}	8	0, 0.3004, 0.4915, 1.3204, 2.2391, 2.8258, 4.3623, 4.4605		9.7762
U_{103}	8	0, 0.5188, 0.6571, 1, 2.3111, 2.5293, 4.1701,	4.8136	9.8776
U_{104}	8	0, 0.4915, 0.6228, 1.3204, 1.7261, 2.8258, 4.3623, 4.6511		9.8794
U_{105}	8	0, 0.3074, 0.8828, 1, 2.2699, 2.7125, 3.8417,	4.9857	9.8405
U_{106}	8	0, 0.2907, 1, 1, 2, 2.8061, 4, 4.9032		9.8428
U_{107}	8	0, 0.3636, 0.5858, 1.3478, 2, 3.2222, 3.4142,	5.0664	9.8372
U_{108}	8	0, 0.3432, 0.6639, 1.1805, 2.2491, 2.9045, 3.5994, 5.0594		9.8376
U_{109}	8	0, 0.2679, 0.6571, 1, 2.5293, 3, 3.7321, 4.8136		9.7765
U_{110}	8	0, 0.2588, 0.6436, 1.1385, 2.1603, 3.1943, 3.8943, 4.7103		9.7788
U_{111}	8	0, 0.2183, 1, 1, 1.7127, 3.5524, 4, 4.5166		9.7859
U_{112}	8	0, 0.2509, 0.7287, 1, 2.3349, 3, 4, 4.6855		9.7792
U_{113}	8	0, 0.2434, 0.6972, 1.1798, 2, 3.1386, 4.3028,	4.4383	9.7814
U_{114}	8	0, 0.2023, 1, 1, 2.2472, 3, 3.4527, 5.0979		9.7969
U_{115}	8	0, 0.4965, 1, 1, 1.7356, 3, 3.5767, 5.1912		9.9237
U_{116}	8	0, 0.3820, 0.7639, 1.3820, 2, 2.6180, 3.6180,	5.2361	9.8903
U_{117}	8	0, 0.2652, 0.8350, 1.4524, 2, 2.8415, 3.2984,	5.3075	9.8538
U_{118}	8	0, 0.3820, 0.4711, 2, 2, 2.6180, 3.1674, 5.3615		9.8461
U_{119}	8	0, 0.2538, 0.5472, 1.4689, 2.4066, 3, 3.1504,	5.1732	9.7883
U_{120}	8	0, 0.5858, 0.5858, 1.2679, 2, 3.4142, 3.4142,	4.7321	9.9418
U_{121}	8	0, 0.4679, 0.7369, 1.4843, 1.6527, 3.1826, 3.8794, 4.5962		9.9438
U_{122}	8	0, 0.4384, 1, 1, 2, 3, 4, 4.5616		9.9442
U_{123}	8	0, 0.3095, 1, 1.3820, 1.6703, 3.3297, 3.6180,	4.6935	9.9149
U_{124}	8	0, 0.3547, 0.7089, 1.5498, 2, 2.8407, 3.8349,	4.711	9.9109
U_{125}	8	0, 0.3249, 0.8299, 1.4608, 2, 2.6889, 4.2143,	4.4812	9.9134
U_{126}	8	0, 0.2679, 0.6571, 2, 2, 2.5293, 3.7321, 4.8136		9.8729
U_{127}	8	0, 0.2243, 1, 1.4108, 2, 2.7237, 4, 4.6412		9.8803
U_{128}	8	0, 0.2442, 0.8455, 1.3465, 2.4678, 2.7742, 3.4537, 4.8681		9.8754
U_{129}	8	0, 0.2355, 0.8711, 1.5254, 2, 2.9050, 3.6799,	4.7831	9.8776
U_{130}	8	0, 0.2907, 0.5858, 2, 2, 2.8061, 3.4142, 4.9032		9.8702
U_{131}	8	0, 0.2679, 0.6571, 2, 2, 2.5293, 3.7321, 4.8136		9.8729
U_{132}	8	0, 0.2243, 0.5858, 1.4108, 2.7273, 3, 3.4142,	4.6412	9.8113
U_{133}	8	0, 0.3065, 0.3820, 1.6703, 2.6180, 3, 3.3297,	4.6935	9.8054
U_{134}	8	0, 0.2137, 0.6177, 1.4977, 2.3537, 3, 3.8408,	4.4763	9.8138
U_{135}	8	0, 0.1864, 1, 1, 2.4707, 3, 4, 4.3429		9.8196
U_{136}	8	0, 0.1892, 0.8207, 1.2558, 2.2216, 3.3354, 3.7575, 4.4198		9.8191
U_{137}	8	0, 0.2137, 0,6177, 1.4977, 2.3537, 3, 3.8408,	4.4763	9.8138
U_{138}	8	0, 0.4915, 0.7530, 1.3204, 1.4450, 2.8258, 3.8019, 4.3623		10.001
U_{139}	8	0, 0.3376, 1, 1.2426, 2.4249, 3, 3.4959, 4.4989		9.9758
$U_{14}0$	8	0, 0.2434, 1.1798, 1.3820, 2, 3.1386, 3.6180,	4.4383	9.9498
U_{141}	8	0, 0.1930, 0.9231, 2, 2, 2.7890, 3.5143, 4.5806		9.9134
U_{142}	8	0, 0.1667, 0.7276, 1.6353, 2.6729, 3, 3.5643,	4.2332	9.8524
U_{143}	8	0, 0.5858, 0.5858, 2, 2, 3.4142, 3.4142,	4	10.0547

On the other hand from **(Tables 4-6),** we can easily see that the energy E of $U_{3=}C_4$, U_8=C_5, U_{21}=C_6 and U_{54}=C_7 is maximal among all other unicyclic molecular graphs in the same number of vertices. But for n=8 the unicyclic molecular graph U_{143}=C_8 has energy 9.6568 which is less then energy of U_{140} and U_{142}. Hence among the unicyclic molecular graphs the cycle Cn has maximal energy E for 3 ≤ n ≤ 7 but for n=8 it is not true.

Table 4: Partial proof of the conjecture.

#	n	Adjacency spectrum	E
U_1	3	2, 1, 1	4
U_2	4	2.1701, 0.3111, 1:0000, 1:4812	4.9624
U_3	4	2, 0, 0, 2	4
U_4	5	2.3429, 0.4707, 0, 1:0000, 1:8136	5.6272
U_5	5	2.3028, 0.6180, 0, 1:3028, 1:6180	5.8416
U_6	5	2.2143, 1.0000, 0:5392, 1:0000, 1:6751	6.4286
U_7	5	2.1358, 0.6622, 0, 0:6622, 2:1358	5.5959
U_8	5	2, 0.6180, 0.6180, 1:6180, 1:6180	6.4721
U_9	6	2.5141, 0.5720, 0, 0, 1, 2:0861	6.1723
U_{10}	6	2.4458, 0.7968, 0, 0, 1:3703, 1:8723	6.4852
U_{11}	6	2.4142, 0.6180, 0.6180, 0:4142, 1:6180, 1:6180	7.3006
U_{12}	6	2.3799, 1, 0.2914, 0:7510, 1, -1.9202	7.3725
U_{13}	6	2.2882, 0.8740, 0, 0, 0:8740, 2:2882	6.3246
U_{14}	6	2.2784, 1.3174, 0, 0:7046, 1, 1:8912	7.1917
U_{15}	6	2.3342, 1.0996, 0.2742, 5945, 1:3738, 1:7397	7.416
U_{16}	6	2.2470, 0.8019, 0.5550, 0:5550, 0:8019, 2:2470	7.2078
U_{17}	6	2.2361, 1, 0, 0, 1, 2:2361	6.4721
U_{18}	6	2.2283, 1.3604, 0.1859, 1, 1, 1:7746	7.5492
U_{19}	6	2.1753, 1.1260, 0, 0, 1:1260, 2:1753	6.6027
U_{20}	6	2.1149, 1, 0.6180, 0:2541, 1:6180, 1:8608	7.4659
U_{21}	6	2, 1, 1, 1, 1, 2	8
U_{22}	7	2.6113, 0.6421, 0, 0, 0, 1, 2:3234	6.6468
U_{23}	7	2.5944, 0.9159, 0, 0, 0, 1:3883, 2:1220	7.0206
U_{24}	7	2.5616, 1, 0, 0, 0, 1:5616, 2	7.1231
U_{25}	7	2.5374, 0.8493, 0.6180, 0, 04891, 1:6180, 1:8976	8.0095
U_{26}	7	2.5450, 1, 0.4394, 0, 0:8302, 1, 2:1542	7.9688
U_{27}	7	2.4495, 1, 0, 0, 0, 1, 2:4495	6.899
U_{28}	7	2.4309, 1.3269, 0.3011, 0, 1, 1, 2:0590	8.1179
U_{29}	7	2.6368, 1.5262, 0, 0, 0:7877, 1, 2:1071	7.7896
U_{30}	7	2.4745, 1.1143, 0.5241, 0, 0:7615, 1:3891, 1:9624	8.2259
U_{31}	7	2.4676, 1.1883, 0.3867, 0, 0:6043, 1:5274, 1:9108	8.0851
U_{32}	7	2.3761, 1, 0.5952, 0, 0:5952, 1, 2:3761	7.9425
U_{33}	7	2.3583, 1.1994, 0, 0, 0, 1:1994, 2:3583	7.1153
U_{34}	7	2.4383, 1.1386, 0.6180, 0, 0:8202, 1:6180, 1:7566	8.3898
U_{35}	7	2.3799, 1.4142, 0.2914, 0, 0:7510, 1:4142, 1:9202	8.1709
U_{36}	7	2.3344, 1, 0.7420, 0, 0:7420, 1, 2:3344	8.1528
U_{37}	7	2.3894, 1.3668, 0.3944, 0, 1, 1:1852, 1:9653	8.3011
U_{38}	7	2.4142, 1, 1, 0:4142, 1, 1, 2	8.8284
U_{39}	7	2.3244, 1.1472, 0.5304, 0, 0:5304, 1:1472, 2:3244	8.0038
U_{40}	7	2.2562, 1.1899, 0.6180, 0, 0:3565, 1:6180, 2:0896	8.1283
U_{41}	7	2.3623, 1.2470, 0.8258, 0:4450, 0:6796, 1:5085, 1:8019	8.8702
U_{42}	7	2.3429, 1.4142, 0.4707, 0, 1, 1:4142, 1:8136	8.4556
U_{43}	7	2.2970, 1.4933, 0.6400, 0:4631, 1, 1, 1:9672	8.8606
U_{44}	7	2.2533, 1.6449, 0.2327, 0, 1, 1:2033, 1:9275	8.2616
U_{45}	7	2.2764, 1.1859, 0.6416, 0, 0:6416, 1:1859, 2:2764	8.2078
U_{46}	7	2.2638, 1.2793, 0.4883, 0, 0:4883, 1:2793, 2:2638	8.0629
U_{47}	7	2.2361, 1.4142, 0, 0, 0, 1:4142, 2:2361	7.3006
U_{48}	7	2.1987, 1.2470, 0.7135, 0, 0:4450, 1:8019, 1:9122	8.3184
		9	

Table 5 : Partial proof of the conjecture.

#	n	Adjacency spectrum	E
U_{49}	7	2.2143, 1, 1, 0, 0:5392, 1:6751, 2	8.4286
U_{50}	7	2.2332, 1.5643, 0.6729, 0:3647, 1, 1:2724, -1.8333	8.9408
$U_5$1	7	2.1889, 1.4142, 0.4569, 0, 0:4569, 1:4142, 2:1889	8.1199
U_{52}	7	2.1515, 1.2685, 0.6180, 0.4206 , 0:8958, 1:6180, 1:9449	8.9174
U_{53}	7	2.1010, 1.2593, 1, 0, 1, 1:2593, 2:1010	8.7206
U_{54}	7	2, 1.2470, 1.2470, 0:4450, 0:4450, 1:8019, 1:8019	8.9879
U_{55}	8	2.8434, 0.6932, 0, 0, 0, 0, 1, 2:5366	7.0732
U_{56}	8	2.7448, 1, 0, 0, 0, 0, 1:3959, 2:3489	7.4896
U_{57}	8	2.6872, 1.1408, 0, 0, 0, 0, 1:6396, 2:1885	7.6561
U_{58}	8	2.6691, 1, 0.6180, 0, 0, 0:5240, 1:6180, 2:1451	8.5742
U_{59}	8	2.6412, 1, 0.7237, 0, 0, 0:5892, 1:7757, 2	8.27298
U_{60}	8	2.6131, 1.0824, 0, 0, 0, 0, 1:0824, 2:6131	7.391
U_{61}	8	2.7073, 1, 0.5359, 0, 0, 0:8719, 1, 2:3713	8.4864
U_{62}	8	2.4860, 1.6636, 0, 0, 0, 0:8360, 1, 2:3136	8.2992
U_{63}	8	2.5178, 1.1380, 0.6045, 0, 0, 0:6045, 1:1380, 2:5178	8.5206
U_{64}	8	2.4972, 1.3281, 0, 0, 0, 0, 1:3281, 2:4972	7.6506
U_{65}	8	2.5860, 1.3350, 0.4559, 0, 0, 1, 1:1317, 2:2453	8.7539
U_{66}	8	2.6095, 1.2598, 0.4468, 0, 0, 0:6084, 1:5710, 2:1367	8.6322
U_{67}	8	2.6200, 1.1311, 0.6634, 0, 0, 0:8339, 1:3962, 2:1843	8.8289
U_{68}	8	2.5009, 1.5558, 0.3044, 0, 0, 1, 1:1401, 2:2208	8.7223
U_{69}	8	2.4812, 1.1701, 0.6889, 0, 0, 0:6889, 1:1701, 2:4812	8.6804
U_{70}	8	2.4495, 1.4142, 0, 0, 0, 0, 1:4142, 2:4495	7.7274
U_{71}	8	2.5831, 1.2346, 0.6180, 0, 0, 0:7631, 1:6180, 2:0545	8.8713
U_{72}	8	2.5553, 1.1946, 0.7799, 0, 0, 0:8911, 1:7177, 1:9210	9.0596
U_{73}	8	2.4495, 1, 1, 0, 0, 1, 1, 2:4495	8.899
U_{74}	8	2.4412, 1.2124, 0.7555, 0, 0, 0:7555, 1:2124, 2:4412	88,182
U_{75}	8	2.5141, 1.4142, 0.5720, 0, 0, 1, 1:4142, 2:0861	9.0006
U_{76}	8	2.4465, 1.6383, 0.2976, 0, 0, 0:8262, 1:4347, 2:1216	8.7649
U_{77}	8	2.4989, 1.4959, 0.4249, 0, 0, 0:7574, 1:6624, 2	8.8395
U_{78}	8	2.5606, 1.1676, 0.6180, 0.5038, 0:3905, 0:8565, 1:6180, 1:9850	9.7
U_{79}	8	2.4728, 1.4626, 0.6180, 0, 0, 1, 1:6180, 1:9354	9.1068
U_{80}	8	2.4142, 1, 1, 0.4142, 0:4142, 1, 1, 2:4142	9.6568
U_{81}	8	2.5714, 1, 1, 0.2754, 0:6379, 1, 1, 2:2116	9.699
U_{82}	8	2.4142, 1.3028, 0.6180, 0, 0, 0:4142, 1:6180, 2:3028	8.67
U_{83}	8	2.4812, 1.1701, 0.6889, 0, 0, 0:6889, 1:1701, 2:4812	8.6804
U_{84}	8	2.5516, 1.3720, 0.5185, 0, 0, 1, 1:2658, 2:1762	8.8841
U_{85}	8	2.4433, 1.5115, 0.6465, 0.2894, 0:5614, 1, 1:2249, 2:1044	9.7814
U_{86}	8	2.3371, 1.2089, 1, 0, 0, 0:6699, 1:6975, 2:1786	9.092
U_{87}	8	2.3113, 1.4269, 0.7353, 0, 0, 0:5338, 1:8365, 2:1032	8.947
U_{88}	8	2.3761, 1.4142, 0.5952, 0, 0, 0:5952, 1:4142, 2:3761	8.771
U_{89}	8	2.3268, 1.6080, 0, 0, 0, 0, 1:6080, 2:3268	7.8696
U_{90}	8	2.4049, 1.2293, 0.6728, 0.5027, 0:5027, 0:6728, 1:2293, 2:4049	9.6194
U_{91}	8	2.3867, 1.3497, 0.6941, 0, 0, 0:6941, 1:3497, 2:3867	8.861
U_{92}	8	2.3968, 1.2665, 0.8069, 0, 0, 0:8069, 1:2665, 2:3968	8.9404
U_{93}	8	2.3761, 1.4142, 0.5952, 0, 0, 0:5952, 1:4142, 2:4161	8.771
U_{94}	8	2.4615, 0.3370, 1, 0, 0:4750, 1, 1:2118, 2:1118	9.5971
U_{95}	8	2.4048, 1.6628, 0.4231, 0, 0, 1, 1:4446, 2:0461	8.9814
U_{96}	8	2.4943, 1.2898, 0.8539, 0.2621, 0:5812, 0:7701, 1:5625, 1:9863	9.8002
		10	

Table 6: Partial proof of the conjecture.

#	n	Adjacency spectrum	E
U_{97}	8	2.3914, 1.6180, 0.7729, 0, 0:6180, 1, 1, 2:1642	9.5645
U_{98}	8	2.3028, 1.8608, 0.2541, 0, 0, 1, 1:3028, 2:1149	6.134722
U_{99}	8	2.4812, 1.4142, 0.6889, 0, 0, 1:1701, 1:4142, 2	9.1686
U_{100}	8	2.5019, 1.1643, 1, 0.2493, 0:4848, 1, 1:3965, 2:0341	9.8309
U_{101}	8	2.4728, 1.4626, 0.6180, 0, 0, 1, 1:6180, 1:9354	9.1068
U_{102}	8	2.4605, 1.2470, 1, 0.2391, 0:4450, 1, 1:6996, 1:8019	9.8931
U_{103}	8	2.2904, 1.2470, 1, 0.3620, 0:4450, 0:5828, 1:8019, 2:0696	9.7987
U_{104}	8	2.2784, 1.3174, 1, 0, 0, 0:7046, 1:8912, 2	9.1916
U_{105}	8	2.3213, 1.4789, 0.6513, 0, 0, 0:6513, 1:4789, 2:3213	8.903
U_{106}	8	2.3072, 1.5355, 0.5645, 0, 0, 0:5645, 1:5355, 2:3072	8.8144
U_{107}	8	2.3583, 1.1993, 1, 0, 0, 1, 1:1993, 2:3583	9.1152
U_{108}	8	2.3562, 1.2918, 0.7741, 0.4244, 0:4244, 0:7741, 1:2918, 2:3562	9.693
U_{109}	8	2.3278, 1.6942, 0.7897, 0, 0:5017, 1, 1:2320, 2:0779	9.6233
U_{110}	8	2.3920, 1.5739, 0.6852, 0.2715, 0:5010, 1, 1:4339, 1:9877	9.8452
U_{111}	8	2.3577, 1.6931, 0.5273, 0, 0, 1:1628, 1:4708, -1.9445	9.1562
U_{112}	8	2.4035, 1.4835, 0.9277, 0, 0:5022, 0:7790, 1:5934, 1:9401	9.6294
U_{113}	8	2.4442, 1.4421, 0.6180, 0.4165, 0:3239, 1:1497, 1:6180, 1:8292	9.8416
U_{114}	8	2.3920, 1.5739, 0.6852, 0.2715, 0:5010, 1, 1:4339, 1:9877	9.8452
U_{115}	8	2.2361, 1.4142, 1, 0, 0, 1, 1:4142, 2:2361	9.3006
U_{116}	8	2.2922, 1.3281, 0.6852, 0.6180, 0:2448, 0:9109, 1:6180, 2:1500	9.8472
U_{117}	8	2.3344, 1.4142, 0.7420, 0, 0, 0:7420, 1:4142, 2:3344	8.9812
U_{118}	8	2.3583, 1.1993, 1, 0, 0, 1, 1:1993, 2:3583	9.1152
U_{119}	8	2.4227, 1.3726, 1, 0.1765, 0:6500, 1, 1:2897, 2:0321	9.9436
U_{120}	8	2.1935, 1.2950, 1.1935, 0.2950, 0:2950, 1:1935, 1:2950, 2:1935	9.954
U_{121}	8	2.1753, 1.4142, 1.1260, 0, 0, 1:1260, 1:4142, 2:1753	9.431
U_{122}	8	2.1701, 1.4812, 1, 0.3111, 0:3111, 1, 1:4812, 2:1701	9.9248
U_{123}	8	2.2105, 1.5047, 0.6180, 0.5043, 0, 1:1554, 1:6180, 2:0641	9.675
U_{124}	8	2.2427, 1.2858, 1, 0.4410, 0:2266, 1, 1:6895, 2:0534	9.939
U_{125}	8	2.2245, 1.4232, 0.8060, 0.5013, 0:2353, 0:9230, 1:8266, 1:9701	9.91
U_{126}	8	2.2552, 1.5582, 0.6970, 0, 0, 0:6970, 1:5582, 2:2552	9.0208
U_{127}	8	2.2143, 1.6751, 0.5392, 0, 0, 0:5392, 1:6751, 2:2143	8.8572
U_{128}	8	2.2853, 1.4534, 0.6880, 0.4376, 0:4376, 0:6880, 0:4534, 2:2853	9.7286
U_{129}	8	2.2725, 1.4924, 0.7801, 0, 0, 0:7801, 1:4924, 2:2725	9.09
U_{130}	8	2.3028, 1.3028, 1, 0, 0, 1, 1:3028, 2:3028	9.2112
U_{131}	8	2.2882, 1.4142, 0.8740, 0, 0, 0:8740, 1:4142, 2:2882	9.1528
U_{132}	8	2.3028, 1.6180, 1, 0, 0:6180, 1, 1:3028, 2	9.8416
U_{133}	8	2.3163, 1.5794, 1, 0.1346, 1, 1, 1, 2:0303	10.0606
U_{134}	8	2.2623, 1.7571, 0.7790, 0.1832, 0:6696, 1, 1:3234, 1:9886	9.9632
U_{135}	8	2.2429, 1.7928, 0.8048, 0, 0:4354, 1, 1:4573, 1:9478	9.681
U_{136}	8	2.3455, 1.5988, 0.7784, 0.2449, 0:4197, 1:2246, 1:4638, 1:8596	9.9353
U_{137}	8	2.3699, 1.4576, 1, 0.1724, 0:5771, 1, 1:5734, 1:8494	9.9998
U_{138}	8	2.0912, 1.4427, 1.2470, 0.2163, 0:4450, 0:7764, 1:8019, 1:9738	9.9943
U_{139}	8	2.1358, 1.4142, 1, 1.6621, 0:6621, 1, 1:4142, 2:1358	10.4242
U_{140}	8	2.1648, 1.4739, 0.7691, 0.6180, 0:1627, 1:2635, 1:6180, 1:9815	10.0515
U_{141}	8	2.1940, 1.5904, 0.8106, 0, 0, 0:8106, 1:5904, 2:1940	9.19
U_{142}	8	2.2350, 1.6881, 1, 0.1326, 0:7386, 1, 1:4460, 1:8711	10.1114
U_{143}	8	2, 1.4142, 1.4142, 0, 0, 1:4142, 1:4142, 2	9.6568

CONCLUSION

In this paper, our attention was focused on the Laplacian-energy-like invariant and energy of unicyclic molecular graphs with at most n vertices, where $3 \leq n \leq 8$, and on the partial proof of the Conjecture 1.1. We have shown that Laplacian- energy-like invariant of cycle Cn is maximal among all other unicyclic molecular graphs for $3 \leq n \leq 8$, a step towards the proof of the Conjecture 1.1.

REFERENCES

[1] Gutman I **(2005)** Topology and stability of conjugated hydrocarbons: The dependence of total π-electron energy on molecular topology. *J Serbian Chem Society* 70: 441-456.

[2] Perić M, Gutman I, Radić-Perić J **(2006)** The Hückel total π-electron energy puzzle. *Journal of the Serbian Chemical Society* 71: 771-783.

[3] Gutman I **(1992)** Total π-electron energy of benzenoid hydrocarbons. In Advances in the Theory of Benzenoid Hydrocarbons II. *Springer, Berlin, Heidelberg* 29-63.

[4] Graovac A, Gotman I, Trinajstic N **(2012)** Topological approach to the chemistry of conjugated molecules (Vol. 4). Springer Science & Business Media.

[5] Gutman I, Polansky OE **(1986)** Automorphism Groups. In Mathematical Concepts in Organic Chemistry (pp. 108-116). Springer, Berlin, Heidelberg.

[6] Gutman I **(2006)** Chemical graph theory—The mathematical connection. Advances in Quantum Chemistry, 51, pp.125-138.

[7] Lin W, Guo X, Li H **(2005)**. On the extremal energies of trees with a given maximum degree. MATCH Commun. Math. Comput. Chem, 54: 363-378.

[8] Li F, Zhou B **(2005)**. Minimal energy of bipartite unicyclic graphs of a given bipartition. MATCH Commun. Math. Comput. Chem, 54 : 379-388.

[9] Yu A, Lu M, Tian F **(2005)** New upper bounds for the energy of graphs. MATCH Commun. Math. Comput. Chem, 53: 441-448.

[10] Yan W, Ye L **(2005)**. On the maximal energy and the Hosoya index of a type of trees with many pendant vertices. MATCH Commun. Math. Comput. Chem, 53: 449-459.

[11] Indulal G, Vijayakumar A **(2006)** On a pair of equienergetic graphs. MATCH Commun. Math. Comput. Chem, 55: 83-90.

[12] Zhou B **(2006)** Lower bounds for energy of quadrangle-free graphs. MATCH Commun. Math. Comput. Chem, 55, 91-94.

[13] Chen A, Chang WC, Shiu **(2006)**, Energy ordering of unicyclic graphs, MATCH Commun. Math. Comput. Chem., 55: 95–102.

[14] Cvetković DM, Doob M, Sachs H **(1980)** Spectra of graphs: theory and application (Vol. 87). Academic Pr.

[15] Gutman I, Zhou B **(2006)** Laplacian energy of a graph. Linear Algebra and its applications, 414: 29-37.

[16] Liu J, Liu BA **(2008)** Laplacian-energy-like invariant of a graph, MATCH Commun. Math. Comput. Chem, 59: 355-372.

[17] Liu B, Huang ZY **(2011)** A survey on the Laplacian-energy-like invariant, MATCH Com- mun. Math. Comput. Chem, 66: 713-730

[18] Stevanovi´c D, lli´c A, Onisor C, Diudea MV **(2009)** LEL−a newly designed molecular descrip- tor, Acta Chim. Sloven, 56: 410-417.

[19] Gutman I, Zhou B, Furtula B **(2010)** The Laplacian-energy like invariant is an energy like invariant, MATCH Commun. Math. Comput. Chem, 64: 85-96

[20] Gutman I, Markovi´c S, Vesovi´c A, Estrada E **(1998)** Approximating total π-electron energy in terms of spectral moments. A quantitative approach, J. Serb. Chem. Soc., 63: 639–646.

[21] Stevanovi´c D **(2009)** Laplacian-like energy of trees, MATCH Commun. Math. Comput. Chem, 61: 407-417.

[22] Read RC, Wilson RJ **(1998)** An Atlas of Graphs, The Clarendon Press Oxford University Press, NewYork.