Research Paper

Hypoenergetic and Strongly Hypoenergetic trees

Sunita Priya D'Silva
Mathematics Dept., Sahyadri College of Engineering & Management.
Email: sunita.math@sahyadri.edu.in

Abstract

In the past few decades, much scientic research has been focused on how to capture and convert by a theoretical pathway the information encoded in a molecu-lar structure of a chemical compound into one or more numbers used to establish quantitative relationships between structures and properties, biological activities, or other experimental properties. Mathematical representations of a molecule, called Molecular Descriptors, are obtained by a well-speciєd algorithm, and are applied to a dened molecular representation or a well-specied experimental procedure. Molecular descriptors are derived by applying principles from several dierent theories, such as quantum-chemistry, information theory, organic chemistry and graph theory. One such molecular descriptor is the parameter energy of the molecular graph of a conjugated hydrocarbon. The energy E(G) of a graph G is dened as the sum of the absolute values of the eigen values of G.

The motivation for the introduction of the this invariant comes from chemistry, where results on E(G) were obtained already in the 1940's. A graph G with n vertices is said to be "hyperenergetic" if E > 2n-2, and to be "hy-poenergetic" if E(G) < n. In this paper we outline the main hitherto obtained results related to Hypoenergetic and strongly Hypoenergetic trees.

Keywords: Energy of the graphs, Hypoenergetic graphs, strongly Hypoenergetic graphs.

1 Introduction

The energy E(G) of a graph G is dened as the sum of the absolute values of the eigen values of G. If 1, 2, 3,............, n are the eigen values of a graph G of n vertices, then energy of G is given by E(G)= $\sum_{i=1}^{n} |_i|$. A n-vertex graph is said to be Hypoenergetic if E(G) < n and strongly Hypoenergetic if E(G)<n-1. Here we characterize the existence of both Hypoenergetic and strongly Hypoenergetic trees of order n and maximum degree .

2 Hypoenergetic and strongly Hypoenergetic trees

We outline the results for Hypoenergetic and strongly Hypoenergetic trees and study for what conditions of vertices(n) the trees are Hypoenergetic and strongly Hy-poenergetic.

1. For Hypoenergetic trees we have the follow-ing results :

(i) There exist Hypoenergetic trees for any number of vertices and any value of maximum vertex degree , except for the case = 4 and n 2 (mod 4).

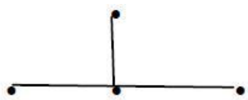
(ii) There exist Hypoenergetic trees of order n with maximum degree 3 only for n = 1, 3, 4, 7.

For e.g.:

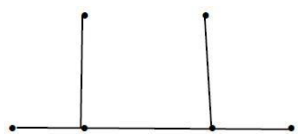
For n=1 S_1: $E(S_1) = 0$.

For n=3 S_3: $E(S_3) = 2.8284$.

For n=4 S_4: $E(S_4) = 3.4640$.



For n=7 G: E(G) = 6.8280.



(iii) If 4, then there exist Hypoenergetic trees for all n + 1.

E.g.: For n = 7 and = 4
G:

2 3
0 1 0 0 0 0 0
61 0 1 0 1 0 17
6 0 1 0 1 0 1 07
6 0 0 1 0 0 0 07
6 0 1 0 0 0 0 07
6 7
0 0 0 0 0 1 0
4 0 1 0 0 0 0 05

The associated matrix is given above and the eigen values are: 2.0743, 0.8350, 1, 0, 0.

The energy of the graph is E(G) = 6.8186 < 7 , so it is hypoenergetic graph.

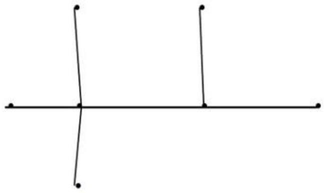
2. For Strongly Hypoenergetic trees we have the following results :

(i) There do not exist Strongly Hypoenergetic trees with maximum degree atmost 3.

(ii)For = 4e, there exist Strongly Hypoenergetic trees for n > 5 such that n 1(mod 4)

Eg: For n = 9 and = 4

G:



21 0 1 0 0 0 1 0 13
0 1 0 0 0 0 0 0 0
6 0 0 1 0 1 0 0 1 07
6 0 1 0 1 0 0 0 0 07
6 0 0 0 1 0 0 0 0 07
6 0 1 0 0 0 0 0 0 07
6 0 0 0 0 0 0 0 0 07
6 0 1 0 0 0 0 0 0 07

4 5

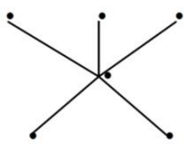
The associated matrix is given above and Eigen values are: 2.829, 1.6673, -1.3417 , -0.3859, 0, 0, 0, 0.

The energy of the graph, E(G) = 7.7005 < 8 =(n - 1), so it is strongly hypoenergetic graph.

(iii) If = 5 , then there exit n vertex strongly hypoenergetic trees for n = 6 and all n â‰¥ 9 but there do not exit any strongly hypoenergetic trees for n = 7 and 8.

Eg: For = 5 and n = 6,

S_6:



2 3
0 1 1 1 1 1
61 0 0 0 0 07
6 1 0 0 0 0 07
6 1 0 0 0 0 07
6 7
1 0 0 0 0 0

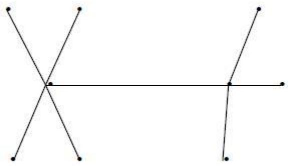
4 1 0 0 0 0 05

The associated matrix for the graph S_6 is given above.

The energy, E(S_6) = 4.4721 < 5 = (n-1), and hence it is strongly hypoenergetic graph.

(iv) For = 5 and n = 9 ,we have the graph G,

G:



21 0 1 0 0 0 0 0 03
0 1 1 1 1 1 0 0 0
61 0 0 0 0 0 0 0 07
1 0 0 0 0 0 0 0 07
61 0 0 0 0 0 1 1 17
60 0 0 0 0 1 0 0 07
60 0 0 1 0 1 0 0 07
6 7
6 7
4 5
0 0 0 0 0 1 0 0 0

The associated matrix is given above and Eigen values are : 2.4495, 1.4142, 0, 0, 0, 0, 0.

The energy, E(G) = 7.7274 < 8 = (n-1), its strongly hypoenergetic graph.

(v) For = 5 and n = 10, we have the graph G

G:

21 0 0 0 0 0 0 0 0 03
0 1 1 1 1 1 0 0 0 0
61 0 0 0 0 0 0 0 0 07
1 0 0 0 0 0 0 0 0 07
60 0 0 0 0 1 0 0 0 07
60 0 0 0 0 1 0 0 0 07
60 0 0 1 0 1 0 0 0 07
6 7
6 7
4 5
0 0 0 0 0 1 0 0 0 0

Eigen values are: 2.5616, 1.5616, 0, 0, 0, 0, 0, 0.

E(G) = 8.2462 < 9 = (n-1), its strongly hypoenergetic graph.

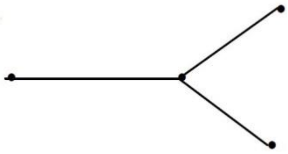
3 Denitions

Nullity: The number of zero eigen values in characteristic equation of the graph is termed as nullity.

Lemma: Let G be a graph with n vertices and m edges. p If nullity of is n0 , then E(G) 2m(n n0).

Note: If the graph is a star, E(G) = 2m(n n0). We have illustrated this below with an example.

Eg: S4:



2 1 0 1 1 3
0 1 1 1
6 0 1 0 0 7
0 1 0 0

4 5

Eigen values are : 1:7321; 0; 0:

N ullity : 2

E(G) = j ij = 3.4642.

p

E(G) = 2 3 (4 2) = 3.4648.

4 Conclusion

We have characterized the trees which are Hypoenergetic and strongly Hypoenergetic with examples using parameters, vertices (n) and maximum degree ( ).

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References

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