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An Analogue of Zagreb Index Inequality Obtained from Graph Irregularity Measures

Asma Hamzeh

Department of Mathematics, Faculty of Mathematical Sciences, Tarbiat Modares University, P.O.Box:14115-137, Tehran, Iran

Tamás Réti[1]

Óbuda University
Bécsi út 96/B, H-1034 Budapest, Hungary

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Abstract: For the structural characterization of a connected graph G with n vertices and m edges two novel graph irregularity measures are introduced, they are defined as $IRM_1(G)=M_1(G)-4m^2/n$ and $IRM_2(G)=M_2(G)-4m^3/n^2$ where $M_1(G)$ and $M_2(G)$ are the first and second Zagreb indices of graph G, respectively. For irregularity indices $IRM_1(G)$ and $IRM_2(G)$ of trees, unicyclic, bicyclic and tricyclic graphs, upper bounds as a function of vertex number n are given. Moreover, it has been proved, that if the Zagreb indices inequality $M_2(G)/m \geq M_1G)/n$ is fulfilled for a connected graph G, then the relation $IRM_2(G)/m \geq IRM_1G)/n$ holds for G, as well. Tests performed on the sets of dual graphs of C_{66} fullerene isomers verified that the topological invariant IRM_2 has a good discriminatory power and can be successfully applicable to the stability prediction of fullerenes.

1. Introduction

Let G=G(V,E) be a simple connected graph with finite vertex set V and edge set E, and denote by $n=|V|$ and $m=|E|$ the number of vertices and edges, respectively. Using the standard terminology in graph theory, we refer the reader to [41]. The degree d(u) of the vertex u is the number of the edges incident to u. Denote by n_i the number of vertices of degree i for i=1,2,..,n-1. The edge of the graph G connecting the vertices u and v is denoted by uv.

[1] Corresponding author. E-mail: reti.tamas@bgk.uni-obuda.hu

Let $\Delta=\Delta(G)$ and $\delta=\delta(G)$ be the maximum and the minimum degrees, respectively, of vertices of G. A graph is called regular, if all its vertices have the same degree. The average degree of a graph G is $[d] = [d(G)] = 2m/n$. A connected graph G is said to be bidegreed with degrees Δ and δ ($\Delta > \delta \geq 1$), if at least one vertex of G has degree Δ and at least one vertex has degree δ, and if no vertex of G has degree different from Δ or δ. A connected bidegreed bipartite graph is called semiregular if each vertex in the same part of a bipartition has the same degree.

Let $g_{n,m}$ denote the family of connected graphs on n vertices and m edges, and let g_n be the class of connected graphs of order n. We shall consider three subclasses of g_n: g_n^1, g_n^2 and g_n^3, which denote the sets of connected unicyclic, bicyclic and tricyclic graphs, respectively. Note that any graph in g_n^1 contains a unique cycle and it has n edges and every graph in g_n^2 contains two linearly independent cycles, having n+1 edges and that any graph in g_n^3 contains three linearly independent cycles, having n+2 edges. Any n-vertex connected graph without cycles is a tree with n-1edges. The girth of G is the length of a shortest cycle contained in G. Let d(u,v) be the length of a shortest path connecting vertices u and v.

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G are defined as [20,21,29,36]:

$$M_1 = M_1(G) = \sum_{u\in V(G)} d^2(u),$$

$$M_2 = M_2(G) = \sum_{uv\in E(G)} d(u)d(v).$$

Conjecture 1 [23] It has been conjectured that for all simple graphs G with n vertices and m edges the so-called Zagreb indices inequality holds, that is,

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m},$$

is fulfilled.

It has been verified that the Zagreb indices inequality is true for a broad class of connected graphs: for chemical graphs with maximum degree four, bidegreed graphs, unicyclic graphs, threshold graphs, graphs with vertex degrees in any interval of length three [1,2,23-27,35,38,40].

Moreover, the bound is tight and is attained if G is a regular or semiregular graph [1,20,21, 27]. It was also shown that there are infinitely many connected graphs, that neither regular nor semiregular, which satisfy the Zagreb indices equality [1].

The Zagreb indices inequality does not hold for general graphs, for example, counter examples are given for connected bicyclic and tricyclic graphs [2,27].

2. Zagreb indices based irregularity indices

In what follows, we define two Zagreb indices based graph irregularity indices. For that purpose, we need the following Lemma:

Lemma 1 [25] Let G be a connected graph. Then $M_1(G) \geq 4m^2/n$ and $M_2(G) \geq 4m^3/n^2$ with equalities if and only if G is a regular graph.

In an analogy with the first and second Zagreb indices, we define the first $IRM_1(G)$ and the second $IRM_2(G)$ *Zagreb irregularity indices* as follows:

$$IRM_1(G) = M_1(G) - \frac{4m^2}{n},$$
$$IRM_2(G) = M_2(G) - \frac{4m^3}{n^2}.$$

From Lemma 1 we can conclude that $IRM_1(G)$ and $IRM_2(G)$ are non-negative numbers and $IRM_1(G) = IRM_2(G)=0$ if and only if G is regular.

Denote by $\sum_2(n,m)$ the maximum value of $M_1(G)$, where G is a connected graph with n vertices and m edges, that is $\sum_2(n,m) = \max\{M_1(G) | G \in g_{n,m}\}$.

Lemma 2 [4] If G is a connected graph on n vertices and m edges such that $M_1(G) = \sum_2(n,m)$, then G contains a vertex of degree n-1.

Sometimes, a vertex u with degree n-1 is called a universal vertex. There are several connected graphs (stars, wheel graphs, windmill graphs, threshold graphs) which contain universal vertices. To select the graphs with a maximum IRM_1 index, by using a computer search, according to Lemma 2, it is enough to consider only the graphs having universal vertices.

Two other closely related measures of graph irregularity are the variance of degree of graph VAR(G) and the Collatz-Sinogowitz index CS(G), which are defined as [6, 7, 22, 30]:

$$VAR(G) = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2 = \frac{1}{n}\sum_{i=1}^{n-1} n_i \left(i - \frac{2m}{n}\right)^2 \geq 0,$$

$$CS(G) = \rho(G) - \frac{2m}{n} \geq 0,$$

where ρ(G) is the spectral radius of graph G. In both cases, equality holds if and only if G is a regular graph. The invariant VAR(G) belongs to the family of degree-based topological indices, which are studied and applied in the mathematical chemistry [15-19,22, 30]. The papers [22, 30] report comparative tests of the irregularity measures VAR(G) and CS(G).

Lemma 3 [30] Let G be a connected graph, then

$$\frac{VAR(G)}{2\sqrt{2m}} \leq CS(G) \leq \sqrt[4]{n^2 VAR(G)}\ .$$

References [37,44] are concerned with vertex degree distributions in unicyclic, bicyclic and tricyclic graphs. The following results will be useful in finding extremal graphs and upper bounds for irregularity indices over such graphs.

A sequence $d_1 \geq d_2 \geq .... \geq d_n$ is called the degree sequence of a graph G if there exists a labeling

$\{v_1, v_2,...,v_n\}$ of vertices of G such that $d_1=d(v_1)$, $d_2 =d(v_2),\ldots, d_n =d(v_n)$.

Lemma 4 [37] Let n ≥3 be an arbitrary positive integer. The integers $d_1 \geq d_2 \geq .... \geq d_n \geq 1$ are the degrees of the vertices of a unicyclic graph if and only if their sum is equal to 2n and at least three of them are greater or equal to 2.

Lemma 5 [37] Let n ≥4 be an arbitrary positive integer. The integers $d_1 \geq d_2 \geq .... \geq d_n \geq 1$ are the degrees of the vertices of a bicyclic graph if and only if their sum is equal to 2n+2 and at least four of them are greater or equal to 2 and $d_1 \leq n - 1$.

Lemma 6 [44] Let n ≥4 be an arbitrary positive integer. Let the integers $n-1 \geq d_1 \geq d_2 \geq .... \geq d_n \geq 1$ be the degrees of the vertices of a tricyclic graph if and only if their sum is equal to 2n+4 and at least four of them are greater or equal to 2 and for sufficiently large n, $(d_1, d_2,..., d_n) \notin \left\{(n-1,\ 4,3,2,1,...,1),(n-1,\ 5,2,2,1,...,1)\right\}$.

Lemma 7 [28] If G is a connected graph that is neither a tree nor a cycle, then the inequality $M_2(G)-M_1(G)\geq 1$ holds.

Lemma 8 [39] For connected graph G, one obtains

$$M_2(G) - M_1(G) = \sum_{uv\in E(G)} \big(d(u)-1\big)\big(d(v)-1\big) - m.$$

The following lemma summarizes some properties of $IRM_1(G)$ and $IRM_2(G)$ irregularity indices.

Lemma 9 Let G be a connected graph with vertex number n and edge number m. Then

$$IRM_1(G) = nVAR(G) = \sum_{i=1}^{n-1} n_i \left(i - \frac{2m}{n} \right)^2 , \tag{1}$$

$$\frac{IRM_1(G)}{2n\sqrt{2m}} \le CS(G) \le \sqrt[4]{nIRM_1(G)} \,. \tag{2}$$

$$\frac{M_2(G)}{m} - \frac{M_1(G)}{n} = \frac{IRM_2(G)}{m} - \frac{IRM_1(G)}{n} \tag{3}$$

Proof. The identities (1) and (3) can be obtained from the definitions of $IRM_1(G)$ and $IRM_2(G)$ indices. The inequality (2) follows directly from Eq. (1) and Lemma 3.■

As a consequence of Eq. (3), one obtains:

Theorem 1. Let G be a connected graph for which the Zagreb indices inequality holds. From Eq. (3) we have

$$\frac{IRM_2(G)}{m} \ge \frac{IRM_1(G)}{n} \tag{4}$$

with equality, for example, if G is regular or semiregular.

3. Irregularity indices of trees, unicyclic, bicyclic and tricyclic graphs

In what follows, we determine the extremal values of $IRM_1(G)$ and $IRM_2(G)$ indices for some particular classes of connected graphs (trees, unicyclic, bicyclic, tricyclic graphs) and additionally, we provide upper bounds for $IRM_1(G)$ and $IRM_2(G)$ indices for connected graphs with arbitrary vertex and edge numbers.

3.1 Irregularity indices of trees

It is known that among n-vertex trees, the path P_n and the star S_n have the minimum and maximum M_1 and M_2 Zagreb indices, respectively [11,20]. From this, it follows that among n-vertex trees the path P_n and the star S_n have the minimum and maximum IRM_1 and IRM_2 indices, respectively.

Lemma 10 [45] If T is a tree on n vertices, then $M_1(T) \leq n(n-1)$ and $M_2(T) \leq (n-1)^2$ and equality holds if and only if T is a star graph S_n.

From Lemma 10 we get:

Theorem 2. Let T be a tree with n vertices and m=n-1 edges. Then

$$IRM_1(T) \leq (n-1)n - \frac{4(n-1)^2}{n} \tag{5}$$

$$IRM_2(T) \leq (n-1)^2 - \frac{4(n-1)^3}{n^2} \tag{6}$$

with equality if and only if T is a star.

Theorem 3 Let T be an n-vertex chemical tree with maximum degree 4. Then

$$IRM_1(T) \leq \begin{cases} \frac{1}{n}\left(2n^2 - 2n - 4\right) & \text{if} \quad n \equiv 2 \pmod{3} \\ \frac{1}{n}\left(2n^2 - 4n - 4\right) & \text{othewise} \end{cases}$$

and the bounds are sharp for all such n≥2. Equality is attained if and only if either (i) every vertex of T is of degree 1 or 4 (in which case $n \equiv 2 \pmod 3$), or (ii) one vertex of T has degree 2 or 3, and all other vertices are of degree 1 or 4.

Proof. The result is the direct consequence of the Theorem 4 in [22], by taking into consideration the equality (1).■

Example 1 Three extremal chemical tree graphs with vertex number 12 are depicted in Fig.1. For them, the maximum value of IRM_1 is equal to 59/3=19.6667.

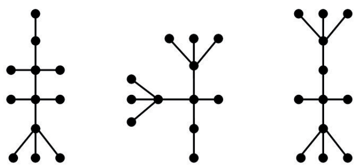


Figure 1: All extremal chemical tree graphs for IRM_1 when n=12

Theorem 4. Let T be an n-vertex chemical tree with maximum degree 4. Then

$$\mathrm{IRM}_2(\mathrm{T}) \leq \begin{cases} 8n - 24 - 4\dfrac{(n-1)^3}{n^2} & \text{if} \quad n \equiv 2 \pmod{3} \\ \\ 8n - 26 - 4\dfrac{(n-1)^3}{n^2} & \text{othewise} \end{cases}$$

with equality if and only if (i) every vertex of T is of degree 1 or 4 (in which case n ≡2 (mod 3)), or (ii) one vertex of T has degree 2 or 3 and it is adjacent to a single vertex of degree 4, while all other vertices are of degree 1 or 4.

Proof. The result follows directly from the Corollary 7 in [17].■

Example 2 In Fig. 2 two extremal chemical tree graphs with vertex number 14 are depicted. For them, the maximum value of IRM_2 is equal to 43.1624.

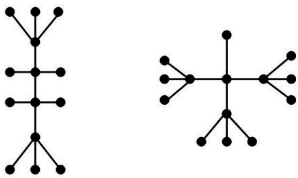


Figure 2: Extremal chemical tree graphs for IRM_2 when n=14

Lemma 11 [35] Let T be a tree with n vertices, m=n-1edges and maximum degree Δ. Then

$$nM_2(T) - mM_1(T) = 0,$$

if T is a star graph, and

$$nM_2(T) - mM_1(T) \geq 2(n-3) + (\Delta-1)(\Delta-2)$$

otherwise. In the above formula, equality is attained if and only if T is a broom.

Recall that a broom is a tree obtained from a star with at least two leaves by replacing one of its edges with a path having at least two edges. From the Lemma 11 one obtains:

Theorem 5. Let T be a tree with n vertices, m=n+1edges and maximum degree Δ. Then

$$IRM_2(T)/m - IRM_1(T)/n = 0,$$

if G is a star graph, and

$$\frac{IRM_2(T)}{m} - \frac{IRM_1(T)}{n} \geq \frac{2(n-3)+(\Delta-1)(\Delta-2)}{nm},$$

otherwise. In the above formula equality holds if and only if T is a broom.

3.2 Irregularity indices of unicyclic graphs

In this section, we obtain results of irregularity indices over unicyclic graphs.

Theorem 6. If G is a unicyclic graph, then $IRM_1(G) \leq n^2 - 5n + 6$ and equality holds if and only if G is isomorphic to $K_{1,n-1}$ + e.

Proof. Since the sum of degrees in G is equal to 2n by Lemma 4, $M_1(G)$ attains its maximum on g_n^1 if and only if d_1=n-1, d_2=d_3=2 and d_4 =…=d_n=1, i.e. G=$K_{1,n-1}$ + e. Therefore, $M_1(G) \leq n^2 - n + 6$ and $IRM_1(G) \leq n^2 - 5n + 6$.■

Theorem 7. [42] If G is a unicyclic graph with n vertices, then $IRM_2(G) \leq n^2 - 4n + 3$ and equality holds if and only if G is isomorphic to $K_{1,n-1}$ + e. Additionally, it has been proved that $K_{1,n-1}$ + e is the unique graph with largest Zagreb index M_2 among all unicyclic graphs with n vertices.

From Lemma 7 and Lemma 8, one obtains directly:

Theorem 8. Let G be a connected unicyclic graph that is not a cycle C_n. Then

$$\frac{IRM_2(G)}{m} - \frac{IRM_1(G)}{n} = \frac{M_2(G)}{n} - \frac{M_1(G)}{n} = -1 + \frac{1}{n}\sum_{uv \in E(G)}(d(u)-1)(d(v)-1)) \geq \frac{1}{n}.$$

It is easy to see that the equality holds for infinitely many connected unicyclic graphs obtained by attaching a pendent edge to a cycle C_n on n≥3 vertices.

3.3 Irregularity indices of bicyclic graphs

In this section, we obtain results concerning irregularity indices over bicyclic graphs.

Theorem 9. If G is a bicyclic graph, then $IRM_1(G) \leq n^2 - 5n + 6 - 4/n$, and equality holds if and only if G is isomorphic to $K_{1,n-1}$ + e + f, where edges e and f meet at a common vertex forming two adjacent triangles. (See Fig 3.)

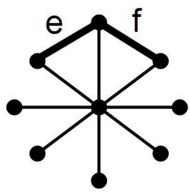


Figure 3: Construction of a bicyclic graph, $K_{1,n-1} + e + f$ (case of n=9)

Proof. Since the sum of degrees in G is equal to 2n + 2 by Lemma 5, $M_1(G)$ attains its maximum on g_n^2 if and only if d_1=n-1, d_2=3, d_3=d_4=2 and d_5 =...= d_n=1, i.e. G = $K_{1,n-1} + e + f$. Therefore, $M_1(G) \le n^2 - n + 14$ and $IRM_1(G) \le n^2 - 5n + 6 - 4/n$. ■

Theorem 10.[12] Let G be an n-vertex bicyclic graph. Then $IRM_2(G) \le n^2 - 2n - 3 - 12/n - 4/n^2$, and equality holds if and only if G is isomorphic to $K_{1,n-1} + e + f$. Moreover, it has been proved that $K_{1,n-1} + e + f$ is the unique graph with largest Zagreb index M_2 among all bicyclic graphs with n vertices.

3.4 Irregularity indices of tricyclic graphs

In this section, we obtain results of irregularity index $IRM_1(G)$ over tricyclic graphs.

Theorem 11. If G is a tricyclic n-vertex graph, then $IRM_1(G) \le n^2 - 5n + 8 - 16/n$, and equality holds only in two cases, that is for two different graphs denoted by H_a and H_b (See Fig 4.):

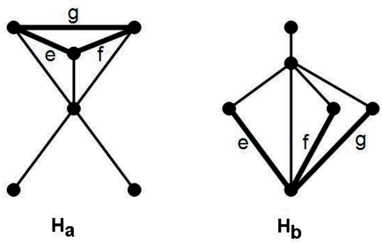


Figure 4: Construction of extremal tricyclic graphs H_a and H_b with two different methods

Proof. Since the sum of degrees in G is equal to 2n + 4 by Lemma 6, $M_1(G)$ attains its maximum on g_n^3 if and only if d_1=n-1, d_2=d_3=d_4=3 and d_5 =...= d_n=1, or d_1=n-1, d_2=4, d_3 = d_4

= d_5 =2 and d_6=...= d_n = 1. Therefore, $M_1(G) \le n^2 - n + 24$ and $IRM_1(G) \le n^2 - 5n + 8 - 16/n$.■

The two versions of the n-vertex extremal graphs (H_a and H_b) can be generated from the graph $K_{1,n-1}$ by adding 3 edges to $K_{1,n-1}$.

a) The graph H_a is constructed from a graph $K_{1,n-1}$ such that $H_a = K_{1,n-1} + e + f + g$, where e and f are two edges with a common vertex, f and g are two edges with common vertex and e and g are two edges with common vertex, so that e, f and g form a triangle.
b) The extremal graph H_b is obtained from $K_{1,n-1}$ such that $H_b = K_{1,n-1} + e + f + g$, but in this case the 3 new edges (e,f,g) are added to $K_{1,n-1}$ such that edges e, f and g will meet at a common vertex of degree 4 (See Fig 4.) ■

3.5 Irregularity indices of connected graphs with arbitrary vertex and edge numbers

In this section, some upper bounds are provided for the irregularity indices of connected graphs with arbitrary vertex and edge numbers.

Lemma 12 [8,9,26,45] Let G be a connected graph with n vertices and m edges. Then

$$M_1(G) \le m\left(\frac{2m}{n-1} + n - 2\right) \qquad (7)$$

with equality if and only if G is the complete graph K_n or the star graph S_n.

Theorem 12. Let G be a connected, non-regular graph with n vertices and m edges. Then

$$IRM_1(G) \le m\left(\frac{2m}{n-1} + n - 2\right) - \frac{4m^2}{n} \qquad (8)$$

with equality if and only if G is a star S_n.

Corollary 1 If G is a tree graph, from Theorem 12, as a particular case, the inequality (5) can be obtained: Let T be a tree graph with n vertices and m=n-1 edges. Then

$$IRM_1(T) \le m\left(\frac{2m}{n-1} + n - 2\right) - \frac{4m^2}{n} \le (n-1)n - \frac{4(n-1)^2}{n} \qquad (9)$$

with equality if and only if T is a star S_n .

Lemma 13. [5,26,45] Let G be a connected graph with n vertices and m edges. Then

$$M_2(G) \le m\left(\sqrt{2m + \frac{1}{4}} - \frac{1}{2}\right)^2 \qquad (10)$$

with equality if and only if G is identical to the complete graph K_n.

As a consequence of Lemma 13, one obtains:

Theorem 13. Let G be a connected graph with n vertices and m edges, different from tree graphs. Then

$$IRM_2(G) \leq m\left(\sqrt{2m+\frac{1}{4}}-\frac{1}{2}\right)^2 - \frac{4m^3}{n^2}. \qquad (11)$$

Remark 1 Several upper bounds for the second Zagreb index of connected graphs are known [5,8,9,26,45]. Comparing these upper bounds, we concluded that the inequality (10) seems to be the best choice. It is easy to see that for tree graphs the inequality (6) can be considered a better upper bound of IRM_2 than the more general inequality represented by Eq. (11).

4. Application: Structural characterization of fullerenes

According to the traditional definition, fullerenes are all-carbon molecules that are modeled by trivalent polyhedra having only pentagonal and hexagonal faces, or simple (3-regular) polyhedral graphs. The vertices represent the carbon atoms, the edges correspond to bounds between pairs of carbon atoms. A fullerene (fullerene graph) with k vertices, denoted by C_k exists for all even $k \geq 20$ except $k=22$, where the number of pentagon is 12, and the number of hexagons is $k/2-10$ [13]. Over the past decade, as a result of intensive research, several quantitative methods have been proposed for the structural characterization of fullerenes. Primarily, for the prediction of their relative stability, a number of graph theoretical invariants (called molecular descriptors) have been defined and studied [14,32,33,34].

In what follows, it will be demonstrated that to the topological classification (stability ranking) of fullerene isomers, certain appropriately defined irregularity indices can also be successfully applicable if we used them for the structural characterization of bidegreed duals of fullerene graphs.

In the set of C_k fullerenes, each isomer has 12 pentagonal faces. Because k is fixed, it follows that the dual graphs of isomers (C_k^{dual}) have 12 vertices of degree 5 and $k/2$ -10 vertices of degree 6, exactly. Consequently, by means of $IRM_1(G)$ irregularity index, it is not possible to discriminate between the graphs (dual graphs) of fullerene isomers having an identical vertex number. It has been expected that the irregularity index $IRM_2(G)$ is more sensitive to the graph structure, and among dual graphs of isomers a better discriminating ability can be achieved.

To test the discriminating power of IRM_2 index, for that purpose, the set of C_{66} isomers has been chosen. The number of topologically different C_{66} isomers is 4478 [32,43] .

Simultaneously, based on the Density Functional Tight-Binding (DFTB) method [31] we calculated the total energy values TQ characterizing the relative stability of isomers. The most stable isomers are characterized by the lowest value of this energy.

Denoting by $\left|V(C_k^{dual})\right|$ and $\left|E(C_k^{dual})\right|$ the number of vertices and edges of dual graphs, for the dual graph C_k^{dual} of a traditional fullerene isomer C_k, the following equalities hold: $\left|E(C_k^{dual})\right| = 3k/2$, $\left|V(C_k^{dual})\right| = (k+4)/2$ and $M_2(C_k^{dual}) = 54k + Np - 360$.

In the above formula, Np stands for the so-called pentagon adjacency index of a fullerene isomer [3,10,13]. This non-negative integer is identical to the total number of edges between adjacent pentagons in a fullerene isomer. It is generally supposed that fullerenes which minimize N_P are more likely to be stable than those that do not [3,10]. For simplicity, let us denote by IRMd the irregularity index of a dual fullerene graph C_k^{dual}. Using the above formulas, for a traditional k-vertex fullerene isomer C_k, one obtains:

$$IRMd = IRM_2(C_k^{dual}) = M_2(C_k^{dual}) - \frac{4\left|E(C_k^{dual})\right|^3}{\left|V(C_k^{dual})\right|^2} = M_2(C_k^{dual}) - \frac{54k^3}{(k+4)^2},$$

This implies that

$$IRMd = 54k + Np - 360 - \frac{54k^3}{(k+4)^2}.$$

As can be seen, for a fixed vertex number k, the irregularity index IRMd can be computed as an increasing linear function of Np. That means that for classical fullerenes the discriminating power of IRMd and Np is considered to be equivalent. In Figure 5, the variation of tight binding total energy (TQ) with IRMd index in C_{66} fullerene isomers is depicted.

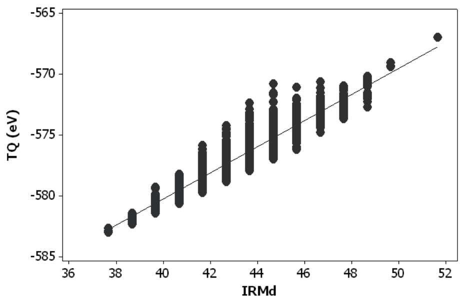


Figure 5: Relation between the tight binding total energy and the IRMd irregularity index

As can be observed, the 4478 isomers form 14 well-separated clusters in the figure. They correspond to the isomer subsets having identical pentagon adjacency indices Np. Consequently, the first cluster represents the most stable 3 isomers, namely C_{66}:4169, C_{66}:4348 and C_{66}:4466 with Np=2. This finding is compatible with the theoretical computational results in [31,43]. There are no isomers corresponding to Np=15. The last cluster belongs to the lonely, “least stable” isomer C_{66}:1 characterized by the maximum pentagon adjacency index (Np=16).

As we can conclude, IRMd can be considered as a quantitative measure of the structural heterogeneity of fullerene isomers, because IRMd characterizes the irregularity in the local arrangement of pentagonal and hexagonal faces. It is worth noting that a particular advantage of IRMd index is that its application can be extended to the structural characterization of non-traditional fullerenes including square and heptagonal faces.

5. Final remarks

We determined the maximum $IRM_2(G)$ indices for connected graphs with n=4, 5 and 6 vertices. The results obtained are included in Table 1.

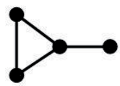
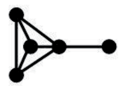
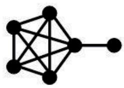
Vertex number, n	Number of n-vertex graphs	Extremal n-vertex graph	$IRM_2(L_n)$
4	6		3.00
5	21		12.12
6	112		33.11

Table 1: Extremal $IRM_2(G)$ index for connected graphs with n=4, 5 and 6 vertices

Based on computed results, it is conjectured that among n≥4-vertex connected graphs the maximum value of the irregularity index $IRM_2(G)$ belongs to the so-called lollipop graphs L_n obtained as by a joining a complete graph K_{n-1} to graph P_2 with a bridge, (that is $L_n = K_{n-1}+e$).

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