Iranian J. Math. Chem. 11 (1) March (2020) 33 − 42

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

Some New Results on Mostar Index of Graphs

MODJTABA GHORBANI•, SHAGHAYEGH RAHMANI AND MOHAMMAD JAVAD ESLAMPOOR

Department of Mathematics, Faculty of Science, Shahid Rajaee, Teacher Training University, Tehran, 16785 – 136, I. R. Iran

ARTICLE INFO

Article History:

Received: 25 November 2019
Accepted: 7 February 2020
Published online: 30 March 2020
Academic Editor: Akbar Ali

Keywords:

Automorphism group
Mostar index
Molecular graphs

ABSTRACT

A general bond additive index can be defined as GBA(Γ)=$\Sigma_{e\in E}$ $\alpha(e)$, where $\alpha(e)$ is the edge contributions. The Mostar index is a new topological index whose edge contributions are $\alpha(e)=|n_u - n_v|$ in which n_u is the number of vertices of Γ lying closer to vertex u than to vertex v and n_v can be defined similarly. In this paper, we propose some new results on the Mostar index based on the vertex-orbits under the action of automorphism group. In addition, we detrmined the structures of graphs with Mostar index equal 1. Finally, we compute the Mostar index of a family of nanocone graphs.

1. INTRODUCTION

All graphs considered in this paper are simple and connected. We refer to [2] for graph theoretical notation and terminology not described here.

Choose an arbitrary edge $e=ab$ of a graph Γ and define $n_a=n(a|\Gamma)$ to be the number of vertices closer to the vertex a than vertex b, see [21]. A long time known property of the Wiener index is the formula [22]:

$$W(\Gamma)=\sum_{e=uv\in E(G)} n(u\mid\Gamma)n(v\mid\Gamma).$$

The Wiener number or Wiener index was proposed in 1947 by the American physical chemist Harold Wiener [22] in which he reported the existence of correlations between the new index and a large number of physical and chemical properties of alkanes such as

•Author to whom correspondence should be addressed (E-mail: mghorbani@sru.ac.ir).
DOI: 10.22052/ijmc.2020.209321.1475

structural determination of paraffin boiling points. This formula is also applicable for trees [12]. This work was considered by a whole series of papers, in all of them, the same quantity has been studied and referred to by scientists [5].

Hosoya [16] in 1971, was the first to conceive the relation between W and the distances in the molecular graph. He, in particular, pointed out the W is equal to

$$W(\Gamma)=\frac{1}{2}\sum_{e=uv\in E(G)} d(u,v),$$

where $d(u,v)$ denotes the length of shortest path connecting two vertices u and v. The Wiener index obtained wide attention and numerous results have been worked out. It has noteworthy applications in chemistry [15]. There exist several Wiener-type toplogical indices based on distances between any pair of vertices, see [3]. The chemical applications and mathematical properties of the Wiener inex are well-studied in [20].

Motivated the above formula, Gutman [13,14] introduced a graph invariant, named as the Szeged index, defined by

$$Sz(\Gamma)=\sum_{e\in E(G)} n_u n_v,$$

where Γ is not necessarily connected. The Szeged index has received a lot of attention immediately after its introduction, see [7,13]. In [18] some formulas for the Szeged index of composite graphs were considered. The authors also proved that for all connected graphs, Sz is greater than or equal to the Wiener index. In [6] the author studied the relationship between Wiener index and Szeged index. Recently, some new kinds of Wiener and Szeged indices are defined which received some consideration in the literature, see [1,9,19].

Djoković in [4] gave a characterization of the so-called geodesic subgraphs of hypercubes. Klavžar [17] used the Djoković–Winkler relation to compute the Wiener index of a partial cube by using a cut method. Following their methods, Ghorbani et al. in [10] computed the Wiener and Szeged indices of a class of dendrimers. This method is also a basis of our given results in Section 3.

The Mostar index is defined in [8,11] as follows:

$$\mathrm{Mo}(\Gamma)=\sum_{e\in E(G)} |n_u-n_v|.$$

An action of G on Ω, G is a group and Ω be a non-empty set, denoted by $(G|\Omega)$ induces a group homomorphism φ from G into the symmetric group S_Ω on Ω, where $\varphi(g)^\alpha = g^\alpha$ ($\alpha\in\Omega$). The orbit of an element $\alpha\in\Omega$ is defined as the set of all α^g, $g\in G$ and denoted by α^G. The size of Ω is called the degree of this action. Suppose $\alpha\in\Omega$. The stabilizer of α is defined as $G_\alpha=\{g\in G: \alpha^g=\alpha\}$. Suppose $H=G_\alpha$, then for $\alpha,\beta\in\Omega$ ($\alpha\neq\beta$), H_β is denoted by $G_{\alpha,\beta}$. The orbit-stabilizer theorem implies that $|\alpha^G|.|G_\alpha|=|G|$.

2. THE MOSTAR INDEX OF TREES

In this section, we present some properties of the Mostar index of trees. For every edge $e = uv$ of graph Γ define N_{uv} to be $N_{uv} =\{x\in V\colon d(u,x)=d(v,x)\}$ and $n_{uv}=|N_{uv}|$. An automorphism of graph Γ is a permutation σ on the set of vertices which preserves the edge set, namely for every edge $e=uv$ we have $\sigma(uv)=\sigma(u)\sigma(v)$. The set of all automorphisms of graph Γ denoted by Aut(Γ) under the composition of mappings forms a group. For the automorphism $\alpha\in$Aut(Γ) we define $fix(\alpha)=\{ x\in V\colon \alpha(x)=x\}$ The graph Γ is called vertex-transitive if it has one orbit. We can similarly define an edge-transitive graph.

Example 2.1. It is clear that in a vertex-transitive graph Γ, for every edge $e=uv$ in $E(\Gamma)$, we have $n_u=n_v$ and thus Mo(Γ)=0. On the other hand, if the Mostar index is zero, then for every edge $e=uv$, we have $|n_u-n_v|=0$ which means that $n_u=n_v$ and thus Γ is distance-balanced graph. In the following theorems, we study the conditions that Mo(Γ)=1.

Theorem 2.1. Suppose Γ is a graph with $n\geq 4$ vertices and Mo(Γ)=1. Then Γ has no pendant edge.

Proof. Suppose Γ has a pendent edge $e=uv$ such that v is the pendent vertex. Then $n_v=1$ and $n_u\geq 3$. Hence $|n_u-n_v|\geq 2$ and Mo(Γ) ≥ 2, a contradiction. ∎

Theorem 2.2. Suppose Γ is a graph and Mo(Γ)=1. Then Γ has no cut edge.

Proof. Suppose Γ has a cut edge $e=uv$ and $\Gamma-e$ has two components, such as Γ_1 and Γ_2. Since Γ_1 has no pendant edge, Γ_1 has at least two vertices and an edge $w,u \in \Gamma_1$. Two following cases hold:

Case 1. Assume $|\Gamma_1|=|\Gamma_2|$. One can see that $n_u \geq |\Gamma_2|+1$ and $n_w \leq |\Gamma_1|-1$. So $n_u-n_w\geq|\Gamma_2|+1-|\Gamma_1|+1\geq 2$, a contradiction.

Case 2. Assume $|\Gamma_1|\neq|\Gamma_2|$. If $||\Gamma_1|-|\Gamma_2||\geq 2$, then $|n_u-n_v|\geq||\Gamma_1|-|\Gamma_2||\geq 2$, a contradiction. Now suppose $||\Gamma_1|-|\Gamma_2||=1$. This means that $|\Gamma_1|=|\Gamma_2|+1$ or $|\Gamma_2|=|\Gamma_1|+1$. If $|\Gamma_1|=|\Gamma_2|+1$, then $|n_u-n_v|=1$. Since Mo(Γ)=1, for any arbitrary edge $uv \neq ab \in E(\Gamma)$, we obtain $n_a=n_b$. So $|\Gamma_2|+1 \leq n_u=n_w \leq |\Gamma_1|-1=|\Gamma_2|$, a contradiction. If $|\Gamma_2|=|\Gamma_1|+1$ by a similar argument, we have $|\Gamma_1|+2= |\Gamma_2|+1\leq n_u=n_w\leq|\Gamma_1|-1$, a contradiction.

This completes the proof. ∎

Corollary 2.1. Suppose Γ is a graph and Mo(Γ)=1. Then Γ is not a tree.

Theorem 2.3. Let T be a tree on $n \geq 3$ vertices and maximum degree Δ. Then

$$\mathrm{Mo}(T) \geq 2\Delta(n-3).$$

Proof. Let $e = uv$ be a pendant edge, where deg(u)=1. Then clearly, $|n_u - n_v| = n-2$. Since, T has at least Δ pendant edges, $\mathrm{Mo}(T) \geq \Delta(n-2)$ and there are at least Δ vertices of degree at least 2. Hence, for all edges incident with the pendant edge $f = ab$, we have $|n_a - n_b| = n-4$. Thus, $\mathrm{Mo}(T) \geq \Delta(n-2) + \Delta(n-4)$. ■

Theorem 2.4. If for any $e = uv \in E(\Gamma)$, there is an automorphism $\rho \in Aut(\Gamma)$ such that $\rho(u) = v$ and $\rho(v) = u$, then $\mathrm{Mo}(\Gamma)=0$.

Proof. Since the automorphism group of graph Γ preserves the distance of vertices, then for any $e = uv \in E(\Gamma)$, one can see that $\{n_u, n_v\} = \{n_{\rho(u)}, n_{\rho(v)}\} = \{n_v, n_u\}$. This means that for any $e = uv \in E(\Gamma)$, $|n_u - n_v| = 0$. This yeilds that $\mathrm{Mo}(\Gamma)=0$.

3. MOSTAR INDEX OF NANOCONES

As we showed in the last section, a graph Γ is distance-balanced if and only if $\mathrm{Mo}(\Gamma)=0$. A fullerene is a cubic three connected graph whose faces entirely composed of pentagons and hexagons. It is a well-known fact that among all fullerene graphs, the fullerene graphs C_{20} and C_{60} are vertex-transitive and thus their Mostar index is zero. Here, we reformulate the Mostar index of graphs in terms of orbits of the automorphism group.

Theorem 3.1. Let $E_1,\ldots,E_r$ be the orbits of graph Γ under the action of $Aut(\Gamma)$ on the set $E(\Gamma)$. Then

$$\mathrm{Mo}(\Gamma) = \sum\nolimits_{i=1}^{r} \sum\nolimits_{e_i \in E_i} |E_i| \times |n_{u_i} - n_{v_i}|. \tag{4}$$

Proof. Let $E_1,\ldots,E_r$ be the orbits of graph Γ. For two edges $e=uv$ and $f = ab$ in the same orbit of Γ, one can prove that $\{n_u, n_v\}=\{n_a, n_b\}$. This completes the proof. ■

According to Theorem 6, if for a graph Γ, we have $\mathrm{Mo}(\Gamma)\neq 0$, then there is the orbit Δ and the edge $f=ab\in\Delta$ where $n_a \neq n_b$. In other words, if there exist an edge $f = ab$ where $n_a \neq n_b$, then we have $\mathrm{Mo}(\Gamma) \geq |f^{\mathrm{Aut}(F)}| \times |n_a - n_b|$.

The subgraph H of Γ is isometric, if for any vertices u and v of H $d_H(u,v) = d_G(u,v)$. An isometric subgraph of a hypercube is called partial cube.

For two edges $e=xy$ and $f=uv$ of graph Γ, are said to be in are in Θ relation, if $d_\Gamma(x,u) + d_\Gamma(y,v) \neq d_\Gamma(x,v) + d_\Gamma(y,u)$. This definition was proposed by Djoković–Winkler in [4]. Winkler proved that if Γ is a bipartite graph, then Θ is transitive and so the relation Θ partitions the set of edges. For the partial cube Γ and its partition F, set $n_1(F)=|\Gamma_1(F)|$

$n_2(F)=|\Gamma_2(F)|$, where $\Gamma_1(F)$ and $\Gamma_2(F)$ are respectively the connected components of $\Gamma\backslash F$. The following theorem proved by Klavžar in [18].

Theorem 3.2. By above notation, for the partial cube Γ, we have

$$\mathrm{W}(\Gamma)=\sum_{F\in H} n_1(F)n_2(F) \text{ and } Sz(\Gamma)=\sum_{F\in H}|F|n_1(F)n_2(F).$$

Corollary 3.1. Let Γ be a partial cube and H its Θ-partition. Then

$$\mathrm{Mo}(\Gamma)=\sum_{F\in H}|F|\times|n_1(F)-n_2(F)|.$$

Here, we compute the Mostar index of an infinite family of nanocones. The relation Θ is always reflexive and symmetric but in general, it is not transitive. The transitive closure of Θ is denoted by Θ^*. In [18] it is proved that all edges of an odd cycle are in the same Θ^*-class.

Definition 3.1. Suppose $F_1,...,F_k$ are the Θ^*-classes of graph Γ. Quotient graphs Γ/F_i, $i=1,...,k$ are defined as a graph with vertex set, the connected components of $\Gamma-F_i$ and two vertices V and V' being adjacent if there exist vertices $x\in V$ and $y\in V'$ such that $xy\in F_i$.

Theorem 3.3. Let Γ be a connected graph with Θ^*-classes $F_1,...,F_k$. Let the quotient graph Γ/F_i, $(i=1,...,k)$, is isomorphic with complete graph K_2 or C_n whose the weight of all vertices are the same. Then all edges of F_i have the same contribution in Mostar index of Γ.

Proof. Suppose $\Gamma/F_i\cong K_2$, this means that $\Gamma-F_i$ has two components C_1 and C_2. Suppose $e=uv$ is an arbitrary edge of F_i such that $u\in C_1$ and $v\in C_2$. It is not difficult to see that $n_u=|C_1|$ and $n_v=|C_2|$. This means that all edges in F_i have the same contribution in computing the Mostar index. Now let $\Gamma/F_i\cong C_n$ and $\Gamma-F_i$ has n components $C_1,...,C_n$. Consider $e=uv$ in F_i, such that $u\in C_i$ and $v\in C_{i+1}$. If n is even, then

$$N_u=C_i\cup C_{i-1}\cup...\cup C_{i-(\frac{n}{2}-1)},$$

and

$$N_v=C_{i+1}\cup C_{i+2}\cup...\cup C_{i+(\frac{n}{2}-1)},$$

where the indices are computed in modulo n. If n is odd, then

$$N_u=C_i\cup C_{i-1}\cup...\cup C_{i-(\frac{n-1}{2}-1)},$$

and

$$N_v=C_{i+1}\cup C_{i+2}\cup...\cup C_{i+(\frac{n-1}{2}-1)},$$

where the indices are computed in modulo n. Since $|C_i|=|C_j|\,(1\le i, j\le n)$, all edges in F_i have the same contribution in computing the Mostar index. ■

Example 3.1. Consider the graph depicted in Figure 1. Consider for example the edge cut F_1, where the edges are colored by green. It is clear that $|F_1|$=15 and thus for the edge $e = uv$ in F_1, we have n_u=n_v=18 or $|n_u$–$n_v|$=0. By applying Theorem 3.3, one can see that for all edges in this class we have $|n_u$–$n_v|$=0. Continuing this method for all edge cuts yields the values of n_{ui}, n_{vi} and equidistant vertices are as reported in Table 1. This means that

$$\mathrm{Mo}(NCP(3)) = (15\times(18-18)) + 5(4\times(38-7)) + 5(5\times(29-16)) = 945.$$

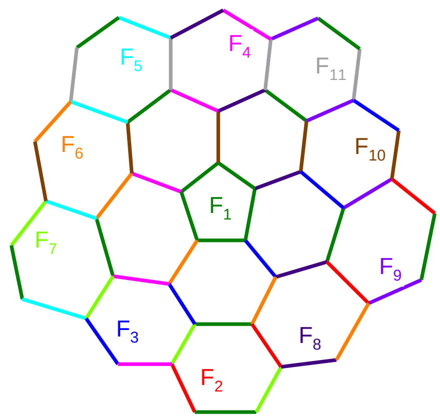

Figure 1. The nanocone $NCP(3)$.

F_i	n_{ui}, n_{vi}, *equidistant*	$\lvert F_i\rvert$
F_1	18,18,9	15
F_2	38,7,0	4
F_3	29,16,0	5
F_4	29,16,0	5
F_5	38,7,0	4
F_6	29,16,0	5
F_7	38,7,0	4
F_8	29,16,0	5
F_9	38,7,0	4
F_0	29,16,0	5
F_{11}	38,7,0	4

Table 1. The values of n_{ui}, n_{vi} and equidistant in nanocone $NCP(3)$.

By a similar way for the graph $NCP(4)$ as depicted in Figure 2, the values of n_{ui}, n_{vi} and equidistant are as reported in Table 2. Thus

$$\begin{aligned} Mo(NCP(4)) &= (20\times(32-32)) + 5(5\times(71-9)) + 5(6\times(60-20)) + 5(7\times(47-33)) \\ &= (5\times5\times62) + (5\times6\times40) + (5\times7\times14) \\ &= 1550+1200+490 = 3240. \end{aligned}$$

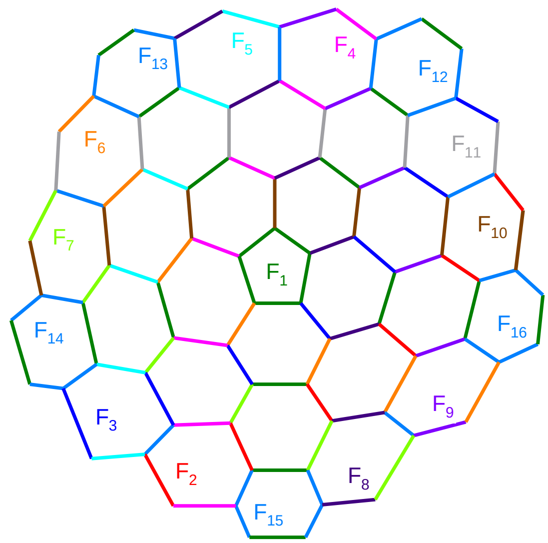

Figure 2. The nanocone $NCP(4)$.

F_i	n_{ui}, n_{vi}, *equidistant*	$\|F_i\|$
F_1	32,32,16	20
F_2	60,20,0	6
F_3	47,33,0	7
F_4	47,33,0	7
F_5	60,20,0	6
F_6	47,33,0	7
F_7	60,20,0	6
F_8	47,33,0	7
F_9	60,20,0	6
F_{10}	47,33,0	7
F_{11}	60,20,0	6
F_{12}	71,9.0	5
F_{13}	71,9.0	5
F_{14}	71,9.0	5
F_{15}	71,9.0	5

F_{16}	71,9.0	5

Table 2. The values of n_{ui}, n_{vi} and equidistant in nanocone $NCP(4)$.

Theorem 3.4. Let $NCP(n)$ be nanocone with $5n^2$ vertices. Then

$$Mo(NCP(n)) = 15n^2(2n^2 - n - 1)/2.$$

Proof. In general, the graph $NCP(n)$ has $5n-4$ Θ^*-classes, such as $F_1,\dots,F_{5n-4}$. By applying Theorem 3.3, the values of n_{ui}, n_{vi} and *equidistant* are as given in Table 3. Hence

$$\begin{aligned} Mo(NCP(n)) &= (5n\times(2n^2-2n^2)) + 5((2n-(n-1))\times(5n^2-2(2n+1))) \\ &\quad + 5((2n-(n-2))\times(5n^2-2(2\times 2n+2^2))) \\ &\quad + \cdots + 5((2n-1)\times(5n^2-2\times(3n^2-4n+1)) \\ &= \sum_{i=1}^{n-1} 25n^3 + 5n^2 i - 30ni^2 - 10i^3 \\ &= \frac{15}{2} n^2(2n^2-n-1). \end{aligned}$$

■

F_i	n_{ui}, n_{vi}, *equidistant*	$\|F_i\|$
$1 \le i \le 5$	$5n^2-(2n+1)$, $2n+1$, 0	$2n-(n-1)$
$6 \le i \le 10$	$5n^2-(4n+4)$, $4n+4$, 0	$2n-(n-2)$
$11 \le i \le 15$	$5n^2-(6n+9)$, $6n+9$, 0	$2n-(n-3)$
.	.	.
.	.	.
.	.	.
$5n-14 \le i \le 5n-10$	$5n^2-(3n^2-8n+4)$, $3n^2-8n+4$, 0	$2n-2$
$5n-9 \le i \le 5n-5$	$5n^2-(3n^2-4n+1)$, $3n^2-4n+1$, 0	$2n-1$
$5n-4$	$2n^2$, $2n^2$, n^2	$5n$

Table 3. The values of n_{ui}, n_{vi} and *equidistant* in nanocone $NCP(n)$.

4. CONCLUSION

In this paper, we showed that the Mostar index of a graph is zero if and only if the graph is distance-balanced. Also, we proved that if Mo(Γ)=1, then Γ is not a tree. In continuing, we obtained some new results about the Mostar index in terms of automorphisms of regarding graph. Finally, we determined the Mostar index of a class of patch fullerenes.

Acknowledgement

This research is partially supported by the Shahid Rajaee Teacher Training University.

REFERENCES

1. J. Bok, B. Furtula, N. Jedlickova and R. Skrekovski, On extremal graphs of weighted Szeged index, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 93–109.
2. J. Devillers and A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Amsterdam, Netherlands, Gordon and Breach, 2000.
3. M. V. Diudea and I. Gutman, Wiener-type topological indices, *Croat. Chem. Acta* **71** (1) (1998) 21–51.
4. D. Djoković, Distance preserving subgraphs of hypercubes, *J. Combin. Theory Ser. B* **14** (1973) 263–267.
5. A. A. Dobrynin, On the Wiener index of certain families of fibonacenes, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 565–574.
6. A. A. Dobrynin, The Szeged and Wiener indices of line graphs, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 743–756
7. A. A. Dobrynin and I. Gutman, On a graph invariant related to the sum of all distances in a graph, *Publ. Inst. Math. Beograd.* **56** (1994) 18–22.
8. T. Došlić, I. Martinjak, R. Škrekovski, S. Tipurić Spužević and I. Zubac, Mostar index, *J. Math. Chem.* (2018), DOI:10.1007/s10910-018-0928-z.
9. M. Ghorbani, X. Li, H. R. Maimani, Y. Mao, S. Rahmani and M. Rajabi-Parsa, Steiner (Revised) Szeged index of graphs, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 733–742.
10. M. Ghorbani; M. Songhori, Some topological indices of nanostar dendrimers, *Iranian J. Math. Chem*. **1** (2010) 57–65.
11. M. Ghorbani and S. Rahmani, A note on Mostar index of a class of fullerenes, *Int. J. of Chem. Model*. 9 (2017) 245–256.
12. I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes N. Y*. **27** (1994) 9–15.
13. I. Gutman and A. A. Dobrynin, The Szeged index-a success story, *Graph Theory Notes N. Y*. **34** (1998) 37–44.

14. I. Gutman, P. V. Khadikar, P. V. Rajput and S. Karmarkar, The Szeged index of polyacenes, *J. Serb. Chem. Soc.* **60** (1995) 759−764.
15. I. Gutman, Y. N. Yeh, S. L. Lee and Y. L. Luo, Some recent results in the theory of the Wiener number, *Indian J. Chem.* **32A** (1993) 651−661.
16. H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated Hydrocarbons, *Bulletin of the chemical society of Journal*, 44 (1971) 2332−2339.
17. S. Klavžar and I. Gutman, A theorem on Wiener-type invariants for isometric subgraphs of hypercubes, *Appl. Math. Lett.* **19** (2006) 1129−1133.
18. S. Klavžar, A. Rajapakse and I. Gutman, The Szeged and the Wiener index of graphs, *Appl. Math. Lett.* **9** (1996) 45-49.
19. X. Li and M. Zhang, A note on the computation of revised (edge-)Szeged index in terms of canonical isometric embedding, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 149−162.
20. G. Rücker and C. Rücker, On topological indices, boiling points and cycloalkanes, *J. Chem. Inf. Comput. Sci.* **39** (1999) 788–802.
21. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
22. H. J. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17−20.