ACADEMIA ROMÂNĂ
Revue Roumaine de Chimie
http://web.icf.ro/rrch/

Rev. Roum. Chim.,
2021, *66*(2), 119-123
DOI: 10.33224/rrch.2021.66.2.02

Papers

Dedicated to Professor Alexandru T. BALABAN
on the occasion of his 90th anniversary

ON DEGREE-AND-DISTANCE-BASED TOPOLOGICAL INDICES

Ivan GUTMAN*

Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia

Received August 6, 2020

In addition to a great variety of degree-based and distance-based molecular structure descriptors, there are a few degree-and-distance-based topological indices. Two main such indices are the degree distance (*DD*) and the Gutman index (*ZZ*). Their mutual relations are analyzed and several new such relations established. It is shown that by conveniently chosen linear combinations of *DD*, *ZZ* and the Wiener index, it is possible to calculate several chemically interesting structural properties of molecular graphs.

$$DD = \sum_{u<v} [d(u) + d(v)]\, d(u,v)$$ degree distance

$$ZZ = \sum_{u<v} [d(u) \cdot d(v)]\, d(u,v)$$ Gutman index

$$DD - ZZ = (n-1)^2$$

INTRODUCTION

In the chemical and mathematical literature, several hundred graph-based molecular structure descriptors were considered, claimed to be related with some physical, chemical, pharmacological, or toxicological property of the underlying compounds. These are usually called "*topological indices*". The vast majority of currently studied topological indices are based on the distances between the vertices of the molecular graph, or on the degrees of the vertices of the molecular graph, or on both.

The oldest distance-based descriptor is the Wiener index.[1] Another among them is the much studied Balaban *J* index.[2] More details on distance-based topological indices can be found in the reviews.[3,4]

The first degree-based structure descriptors were conceived in the 1970s. There are the fist Zagreb index,[5] the second Zagreb index,[6] and the Randić index.[7]

Much later, the first degree-and-distance-based topological indices were put forward.[8-10]

Initially, there was only a small number (less than one dozen) of topological indices.[11] The rapid increase in their number started by a paper by Alexandru T. Balaban[12], in which five new indices were simultaneously introduced. More details on the theory and applications of topological indices can be found in numerous surveys, for instance in the books.[13-15]

DEGREE DISTANCE AND ITS CONGENERS

Let *G* be a molecular graph with *n* vertices, labeled by $v_1, v_2, ..., v_n$. The *degree* of the vertex

* Corresponding author: gutman@kg.ac.rs

v_i, denoted by $d(v_i)$, is the number of its first neighbors. The *distance* between the vertices v_i, v_j, denoted by $d(v_i, v_j)$, is the length of (= number of edges in) a shortest path in the underlying graph,, connecting v_i and v_j Additional notions and definitions on molecular graphs can be found in the reviews[16-18] and books.[19-22]

In this paper, we are concerned with degree-and-distance-based topological indices, of which the most important is the degree distance, *DD*. Before we introduce it, we recall that the classical *Wiener index* is defined as

$$W = W(G) = \sum_{i<j} d(v_i, v_j) \qquad (1)$$

where the summation goes over all pairs of vertices of the underlying molecular graph *G*. The Wiener index was introduced in 1947 by Harold Wiener[1] and since then became one of the most extensively studied distance-based topological indices; for details see.[22-24]

Motivated by the success of the Wiener index, Dobrinin and Kochetova proposed its degree-weighted version, named *degree distance,* defined as

$$DD = DD(G) = \sum_{i<j} [d(v_i) + d(v_j)] d(v_i, v_j) . \quad (2)$$

The degree distance was put forward in 1994. In the meantime, this degree-and-distance-based topological index became a popular topic for mathematical studies and chemical applications; for details see the recent papers[25-28] and the references cited therein. However, five years before the concept of degree distance was conceived, Schultz considered a seemingly unrelated quantity, which he named *molecular topological index*, and defined as[8]

$$MTI = MTI(G) = \sum_{k=1}^{n} \left[\begin{pmatrix} d(v_1 \\ d(v_2) \\ \cdots \\ d(v_n) \end{pmatrix} A + D \right]_k$$

where *A* and *D* denote the adjacency and distance matrices (of the graph *G*). It can be shown that[10]

$$MTI = \sum_{k=1}^{n} d(v_k)^2 + DD .$$

The fact that in the case of acyclic graphs, there is a simple linear relation between *MTI* and the Wiener index was first noticed in[29] and then mathematically proven by Douglas Klein.[30] An independent proof was offered by the present author.[10] All this happened before the publication of the Dobrynin-Kochetova article.[9] The respective result can be stated as:[10,30]

$$DD(T) = 4W(T) - n(n-1) \qquad (3)$$

which holds for any tree *T* with *n* vertices.

The author of the paper[10] noticed that by means of his proof technique, an identity analogous to Eq. (3) can be deduced for the expression in which the sum $d(v_i) + d(v_j)$ is replaced by the product $d(v_i) \cdot d(v_j)$. Thus, for the quantity *ZZ,* defined as,

$$ZZ = ZZ(G) = \sum_{i<j} [d(v_i) \cdot d(v_j)] d(v_i, v_j) \quad (4)$$

the following result could be verified:[10]

$$ZZ(T) = 4W(T) - (2n-1)(n-1) . \qquad (5)$$

The degree-and-distance-based quantity *ZZ* appeared in the paper[10] for the first time. The sole reason for its introduction was to point out the analogy between Eqs. (3) and (5). There was no intention to consider it as a new molecular structure descriptor. No name for it was proposed.

When Todeschini and Consonni produced their "Handbooks of Molecular Descriptors",[14] they mentioned in it the quantity *ZZ* and named it *Gutman index*. This name was eventually accepted in the mathematical and chemical literature, see the recent articles[26,31-35] and the references cited therein. Nevertheless, in the present paper we prefer to avoid using this name, and will call the topological index *ZZ*, Eq. (4), as the *ZZ-index*.

We now introduce the following generalizations of the degree distance, Eq. (2), and the *ZZ*-index, Eq. (4). Let *t* be a real number. Then we define

$$DD_t = DD_t(G) = \sum_{i<j} \Big[[d(v_i) - t] + [d(v_j) - t] \Big] d(v_i, v_j) \qquad (6)$$

and

$$ZZ_t = ZZ_t(G) = \sum_{i<j} \Big[[d(v_i) - t] \cdot [d(v_j) - t] \Big] d(v_i, v_j) . \quad (7)$$

At this point, one should note that in spite of what may be concluded from Eqs. (6) and (7), DD_t and ZZ_t are not new topological indices. Namely, bearing in mind Eqs. (1), (2), and (4), it is elementary to show that for any connected graph G,

$$DD_t(G) = DD(G) - 2t\,W(G) \quad (8)$$

and

$$ZZ_t(G) = ZZ(G) - t\,DD(G) + t^2\,W(G) . \quad (9)$$

Thus, DD_t and ZZ_t are just linear combinations of the previously conceived degree-and-distance based indices *DD* and *ZZ,* and the classical distance-based Wiener index *W*. Nevertheless, in the following two sections we show that by using conveniently chosen special cases of these linear combinations, it is possible to immediately calculate several chemically interesting structural properties of molecular graphs.

APPLICATIONS: RELATIONS BETWEEN *DD*- AND *ZZ*-INDICES OF GRAPHS

A large number of molecular graphs have only vertices of degree two and three. Among these are the molecular graphs of benzenoid systems, phenylenes, fluoranthenes, and numerous other classes of polycyclic conjugated hydrocarbons, both alternant and nonalternant. Some characteristic examples are depicted in Fig. 1.

By $\Gamma(p,q)$ we denote the set of all connected graphs in which all vertex degrees are equal to either p or q.

Let G be a molecular graph belonging to the set $\Gamma(2,3)$. Its Wiener index can be partitioned into three parts, $W(G) = W_{22}(G) + W_{23}(G) + W_{33}(G)$, where $W_{ij}(G)$ for i=1,2, is the sum of distances between vertices of degree i and degree j of the graph G.

Proposition 1. If $G \in \Gamma(2,3)$, then

$$W_{22}(G) = 9W(G) - 3\,DD(G) + ZZ(G) \quad (10)$$

$$W_{23}(G) = 5\,DD(G) - 2\,ZZ(G) - 12\,W(G) \quad (11)$$

$$W_{33}(G) = ZZ(G) - 2\,DD(G) + 4\,W(G) . \quad (12)$$

Proof. Taking into account the definition (7), we see that $ZZ_2(G) = W_{33}(G)$ and by Eq. (9) we directly arrive at relation (12). Analogously, definition (6) implies $DD_2(G) = W_{23}(G) + 2W_{33}(G)$, which by Eq. (8) yields $W_{23}(G) + 2W_{33}(G) = DD(G) - 4W(G)$. Combining this with (12) results in (11). Finally, (10) is obtained by combining $W_{22}(G) = W(G) - W_{23}(G) - W_{33}(G)$ with (11) and (12).

In 1874, Arthur Cayley introduced the concept of molecular graph.[36] He distinguished two types of such graphs, and named them *plerogram* and *kenogram*. In the plerogram, all atoms, including hydrogen atoms, are represented by vertices. In the kenogram, hydrogen atoms are disregarded. Plerograms and kenograms are sometimes referred to as *hydrogen-filled* and *hydrogen-depleted* molecular graphs. An example is given in Fig. 2. The vast majority of contemporary chemical applications of graph theory[13-15,19-22] deals with kenograms.

The plerograms of a saturated hydrocarbons belongs to the set $\Gamma(1,4)$. Then, in analogy to Proposition 1, we have:

Proposition 2. If $G \in \Gamma(1,4)$, then $W(G) = W_{11}(G) + W_{14}(G) + W_{44}(G)$ and

$$W_{11}(G) = \frac{1}{9}\big[14\,W(G) - 4\,DD(G) + ZZ(G)\big] \quad (13)$$

$$W_{14}(G) = \frac{1}{9}\big[5\,DD(G) - 2\,ZZ(G) - 6\,W(G)\big] \quad (14)$$

$$W_{44}(G) = \frac{1}{9}\big[ZZ(G) - DD(G) + W(G)\big] . \quad (15)$$

Proof. Taking into account the definition (7), we see that $ZZ_1(G) = 9\,W_{44}(G)$ and by Eq. (9) we directly arrive at relation (15). Definition (6) implies $DD_1(G) = 3\,W_{14}(G) + 6\,W_{44}(G)$, which by Eqs. (8) and (15) results in Eq. (14), whereas Eq. (13) is obtained by substituting (14) and (15) back into $W_{11}(G) = W(G) - W_{14}(G) - W_{44}(G)$.

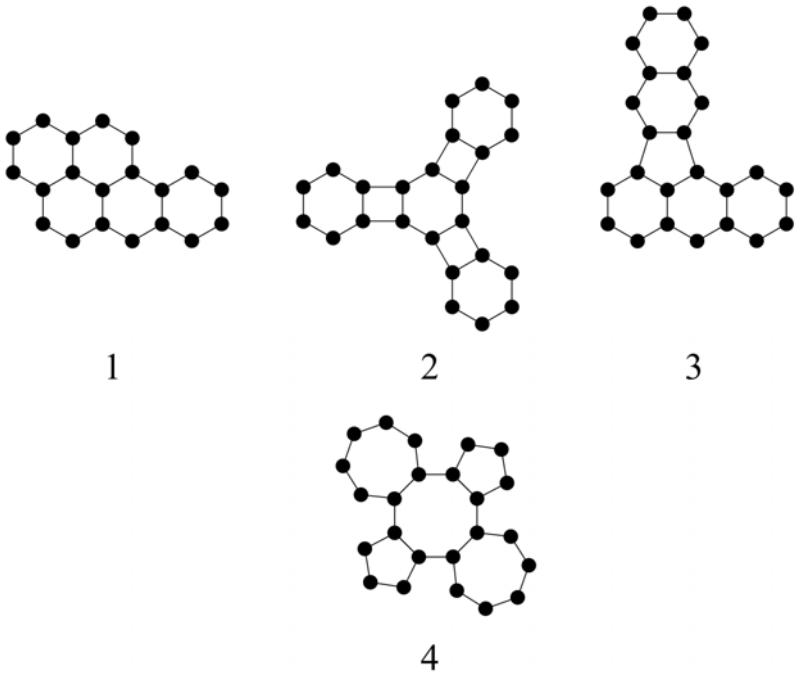

Fig. 1 – Examples of molecular graphs belonging to Γ(2,3): a molecular graph of a benzenoid system (**1**), phenylene (**2**), fluoranthene (3), and bicalicene (4).

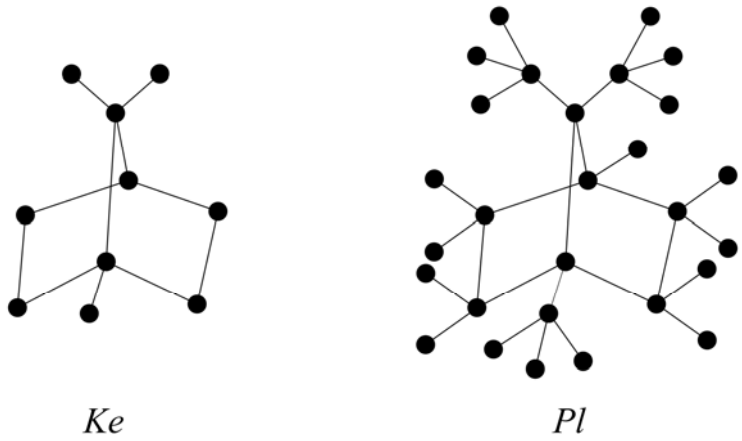

Fig. 2 – The molecular graph of camphene, $C_{10}H_{18}$. *Ke* is its kenogram (hydrogen-depleted graph), in which vertices correspond only to carbon atoms; *Pl* is its plerogram (hydrogen-filled graph), in which vertices correspond to both carbon and hydrogen atoms.

APPLICATIONS: RELATIONS BETWEEN *DD*- AND *ZZ*-INDICES OF TREES

In the case of trees, the fundamental relations for the *DD*- and *ZZ*-indices are Eqs. (3) and (5), known since the 1990s.[10,30] An immediate and remarkable consequence of these relations is the following:

Proposition 3. Let T be a tree with n vertices. Then

$$DD(T) - ZZ(T) = (n-1)^2$$

i.e.,

$$\sum_{i<j} [d(v_i) + d(v_j) - d(v_i) \cdot d(v_j)] d(v_i, v_j) = (n-1)^2 .$$

Thus, the difference between the *ZZ*- and *DD*-indices is independent of the structure of the tree T, and depends only on its size.

In analogy to Proposition 3, we have

$$DD_2(T) = -n(n-1)$$

and

$$ZZ_2(T) = n-1$$

which are obtained by substituting Eqs. (3) and (5) back into (8) and (9).

If the graph G in Proposition 2 is a tree, *i.e.*, if it corresponds to the plerogram of an alkane, then by using Eqs. (3) and (5) we get:

Proposition 4. If $T \in \Gamma(1,4)$ is a tree with n vertices, then

$$W_{11}(T) = \frac{1}{9}\left[2W(T) + (2n+1)(n-1)\right]$$

$$W_{14}(T) = \frac{1}{9}\left[6W(T) - (n+2)(n-1)\right]$$

$$W_{44}(T) = \frac{1}{9}\left[W(T) - (n-1)^2\right]. \qquad (16)$$

If T is the kenogram Ke of an alkane $C_N H_{2N+2}$, then $W(T)$ is the Wiener index of the kenogram, *i.e.*, $W(T) \equiv W(Ke)$. Then $W_{44}(T)$ is the Wiener index of the respective kenogram, *i.e.*, $W_{44}(T) = W(Ke)$. Noting that $n = 3N + 2$, Eq. (16) can be rewritten as $W(Pl) = 9W(Ke) + (3N+1)^2$ a formula that earlier[37] was obtained by a different method.

REFERENCES

1. H. Wiener, *J. Am. Chem. Soc.,* **1947**, *69*, 17–20.
2. A. T. Balaban, *Chem. Phys. Lett.,* **1982***, 89*, 399–404.
3. A. T. Balaban, *Pure Appl. Chem*., **1983**, *55*, 199–206.
4. K. Xu, M. Liu, K. C. Das, I. Gutman and B. Furtula, *MATCH Commun. Math. Comput. Chem***., 2014**, *71*, 461–508.
5. Gutman and N. Trinajstić, *Chem. Phys. Lett*., **1972**, *17*, 535–538.
6. I. Gutman, B. Ruščić, N. Trinajstić and C. F. Wilcox, *J. Chem. Phys*., **1975**, *62*, 3399–3405.
7. M. Randić*, J. Am. Chem. Soc*., **1975**, *97*, 6609–6615.
8. H. P. Schultz, *J. Chem. Inf. Comput. Sci.,* **1989**, *29*, 227–228.
9. A. A. Dobrynin, and A. A. Kochetova, *J. Chem. Inf. Comput. Sci*., **1994**, *34*, 1082–1086.
10. I. Gutman, *J. Chem. Inf. Comput. Sci*., **1994**, *34*, 1087–1089.
11. A. T. Balaban, I. Motoc, D. Bonchev and O. Mekenyan, *Topics Curr. Chem.*, **1983**, *114*, 21–55.
12. A. T. Balaban, *Theor. Chim. Acta*, **1979**, *53*, 355–375.
13. J. Devillers and A. T. Balaban (Eds.), "Topological Indices and Related Descriptors in QSAR and QSPR", Gordon & Breach, Amsterdam, 1999.
14. R. Todeschini and V. Consonni, "Handbook of Molecular Descriptors", Wiley-VCH, Weinheim, 2000.
15. R. Todeschini and V. Consonni, "Molecular Descriptors for Chemoinformatics", Wiley-VCH, Weinheim, 2009.
16. A. T. Balaban, J. *Chem. Inf. Comput. Sci*., **1985**, *25*, 334–343.
17. A. T. Balaban, *J. Mol. Struct. (Theochem),* **1985**, *120*, 117–142.
18. A. T. Balaban, *J. Chem. Inf. Comput. Sci.,* **1995**, *35*, 339–350.
19. A. T. Balaban (Ed.), "Chemical Applications of Graph Theory", Academic Press, London, 1976.
20. I. Gutman and O. E. Polansky, "Mathematical Concepts in Organic Chemistry", Springer, Berlin, 1986.
21. A. T. Balaban (Ed.), "From Chemical Topology to Three-Dimensional Geometry", Plenum Press, New York, 1997.
22. S. Wagner and H. Wang, "Introduction to Chemical Graph Theory", CRC Press, Boca Raton, 2018.
23. A. A. Dobrynin, R. Entringer and I. Gutman, *Acta Appl. Math*., **2001**, *66*, 211–249.
24. M. Knor, R. Škrekovski, A. Tepeh, *Ars Math. Contemp*., **2016**, *11*, 327–352.
25. Y. Alizadeh and S. Klavžar, *MATCH Commun. Math. Comput. Chem*., **2020**, *84*, 647–659.
26. S. Brezovnik and N. Tratnik, *MATCH Commun. Math.. Comput. Chem*., **2019**, *82*, 111–132.
27. I. Redžepović, Y. Mao, Z. Wang and B. Furtula, *Int. J. Quantum Chem.*, **2020**, *120*, #e26209.
28. W. Weng and B. Zhou, *MATCH Commun. Math. Comput. Chem*., **2020**, *84*, 629–645.
29. D. Plavšić, S. Nikolić, N. Trinajstić and D. J. Klein, *Croat. Chem. Acta*, **1993**, *66*, 345–353.
30. D. J. Klein, Z. Mihalić, D. Plavšić and N. Trinajstić, *J. Chem. Inf. Comput. Sci*., **1992**, *32*, 304–305.
31. B. Ali, M. Imran, M. A. Malik, H. M. A. Siddiqui, A. Bilal and M. R. Farahani, *Adv. Appl. Discr. Math*., **2019**, *20*, 165–184.
32. M. An and L. Xiong, *Ars Combin*., **2019**, *143*, 117–134.
33. V. Kaladevi and G. Kavitha, *Int. J. Innov. Technol. Explor. Engin.*, **2019**, *8*, 1982–1989
34. S. Sedghi and N. Shobe, J. *Algebra Comb. Discr. Struct. Appl.*, **2020**, *7*, 121–140.
35. L. Zhang, Q. Li, S. Li and M. Zhang, Discr. *Appl. Math.*, **2020**, *282*, 243–256.
36. A. Cayley, *Philos. Mag.,* **1874**, *47*, 444–446.
37. I. Gutman, D. Vidović, L. Popović, *J. Chem. Soc. Faraday Trans*., **1998**, *94*, 857–860.