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Sombor and KG-Sombor Indices of Benzenoid Systems and Phenylenes

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Abstract. Let d(v) denote the degree of a vertex v, and d(e) the degree of an edge e. The Sombor index SO is a vertex-degree-based (VDB) topological index, equal to the sum of terms $\sqrt{d(u)^2 + d(v)^2}$ over all pairs of adjacent vertices u and v of the underlying molecular graph. Recently a variant of SO was put forward, the KG-Sombor index, KG, equal to the sum of terms $\sqrt{d(u)^2 + d(e)^2}$ where u is an endpoint of the edge e.- In this paper, we give general expressions for SO and KG of benzenoid systems and phenylenes.

Keywords: Topological index, Sombor index, KG-Sombor index, degree (of vertex), degree (of edge), benzenoid system, phenylene

AMS Mathematics Subject Classification (2010): 05C05, 05C07, 05C90

1. Introduction

In the current mathematical and chemical literature, several dozens of vertex-degree-based (VDB) graph invariants (usually referred to as "topological indices") are being considered [1-3].

Their general form is

$$TI(G) = \sum_{uv \in E(G)} F((u), d(v)) \qquad (1)$$

where F is some function having the property $F(x,y)=F(y,x)$. In Eq. (1) and throughout this paper, $d(u)$ is the degree (= number of first neighbors) of the vertex u of the underlying graph G, whereas the summation goes over pairs adjacent of vertices u,v, i.e., over the edges $e=uv$ contained in the edge set $E(G)$ of the graph G.

An edge of the graph G, connecting a vertex of degree i and a vertex of degree j, is called an (i,j)-edge. The number of such edges will be denoted by $m_{i,j}$. Then Eq. (1) can be written as

$$TI(G) = \sum_{1 \le i \le j \le n-1} F(i, j)\, m_{i,j}\,. \qquad (2)$$

One of the newly introduced VDB topological indices is the Sombor index [4]

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2} \tag{3}$$

which recently attracted much attention, see [5-9] and the references cited therein. Motivated by the success of the Sombor index, the present authors examined the possibility of including edge degrees, and defined the KG-Sombor index as [10].

$$KG(G) = \sum_{ue} \sqrt{d(u)^2 + d(e)^2} \tag{4}$$

where the summation goes over all pairs of vertices u and edges e, such that u is an endpoint of e.

If the other endpoint of the edge e is the vertex v, then Eq. (4) can be rewritten according to the form of Eq. (1), namely as [10]:

$$KG(G) = \sum_{uv \in E(G)} \left[\sqrt{d(u)^2 + [d(u) + d(v) - 2]^2} + \sqrt{d(v)^2 + [d(u) + d(v) - 2]^2} \right]. \tag{5}$$

Note that in Eq. (5) we use the fact that the degree of an edge $e=xy$ satisfies the relation $d(e)=d(u)+d(v)$-2.

In this paper, we study the Sombor and KG-Sombor indices of benzenoid systems (cf. Fig. 1) and of phenylenes (cf. Fig. 2). These molecular graphs posess only vertices of degree 2 and 3. Consequently, all their edges are of type (2,2), (2,3), and (3,3). Therefore, for benzenoids and phenylenes, Eq. (2) has the following simple form:

$$TI(G) = F(2,2)m_{2,2} + F(2,3)m_{2,3} + F(3,3)m_{3,3} \tag{6}$$

The values of $F(2,2)$, $F(2,3)$, and $F(3,3)$ for the Sombor and KG-Sombor indices follow immediately from Eqs. (3) and (5), respectively. Thus we have:

	Sombor index	KG-Sombor index
$F(2,2)$	$2\sqrt{2}$	$4\sqrt{2}$
$F(2,2)$	$\sqrt{13}$	$\sqrt{13}+3\sqrt{2}$
$F(2,2)$	$3\sqrt{2}$	10

What remains is no determine the parameters $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ for benzenoid systems and for phenylenes.

2. On structural features and Sombor indices of benzenoid systems

The structural features of benzenoid systems (= molecular graphs of benzenoid hydrocarbons) have been studied in due detail [11,12], see also [13,14]. Their main topological properties are determined by three parameters, namely:

n = number of vertices,
h = number of hexagons, and
r = number of inlets.

The number of inlets is equal to the number of strings of 3-degree vertices on the boundary of the underlying benzenoid system, for details see [13,14. The structural detail determined by the sequence 232 is said to be a "*fissure*". The features pertaining to the sequences 2332, 23332, and 233332, are referred to as "*bay*", "*cove*", and "*fjord*", respectively, see Figure 1.

The edges of a benzenoid system connect either two vertices of degree 2, or two vertices of degree 3, or a vertex of degree 2 with a vertex of degree 3. Thus, its edges are either of type (2,2) or (2,3) or (3,3), noting that all (2,2)- and (2,3)-type edges lie on the boundary. Their numbers are denoted by $m_{2,2}$, $m_{3,3}$, and $m_{2,3}$, respectively, and it is known that [13,14]

$$m_{2,2} = n - 2h - r + 2$$
$$m_{2,3} = 2r$$
$$m_{3,3} = 3h - r - 3$$

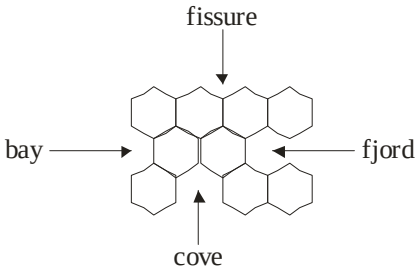

Figure 1: A benzenoid system and the structural details on its boundary. It has 4 fissures, one bay, one cove, and one fjord. Thus its number of inlets is r = 4+1 + 1 + 1 = 7.

Consequently, by using Eq. (6), for any benzenoid system B with n vertices, h hexagons, and r inlets,

$$\begin{aligned} SO(B) &= 2\sqrt{2}(n-2h-r+2)+\sqrt{13}(2r)+3\sqrt{2}(3h-r-3) \\ &= 2\sqrt{2}\,n+5\sqrt{2}\,h+(2\sqrt{13}-5\sqrt{2})\,r-5\sqrt{2} \\ &= 2.828n+7.071(h-1)+0.140r \end{aligned}$$

$$\begin{aligned} KG(B) &= 4\sqrt{2}(n-2h-r+2)+(\sqrt{13}+3\sqrt{2})(2r)+10(3h-r-3) \\ &= 4\sqrt{2}\,n+(30-8\sqrt{2})\,h+(2\sqrt{13}+2\sqrt{2}-10)\,r-(30-8\sqrt{2}) \\ &= 5.657n+18.686(h-1)+0.040r \end{aligned}$$

3. On structural features and Sombor indices of of phenylenes

The molecular graphs of phenylenes consist 6 and 4 membered cycles, so that avery 4-membered cycle is adjacent to two 6-membered cycles (or hexagons) and no two hexagons are adjacent. A characteristic example of a phenylene graph is depicted in Figure 2.

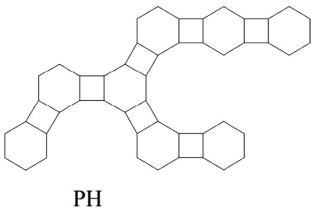

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Figure 2: A phenylene graph.

A phenylene P with h hexagons has $6h$ vertices. It has been shown [13] that for a phenylene with h hexagons and r inlets,

$$m_{2,2} = 2h - r + 4$$
$$m_{2,3} = 2r$$
$$m_{3,3} = 6h - r - 6$$

from which, in view of Eq. (6), it follows:

$$\begin{aligned} SO(P) &= 2\sqrt{2}(2h - r + 4) + \sqrt{13}(2r) + 3\sqrt{2}(6h - r - 6) \\ &= 22\sqrt{2}\,h + (2\sqrt{13} - 5\sqrt{2})\,r - 10\sqrt{2} \\ &= 31.113h + 0.140r - 14.142 \end{aligned}$$

$$\begin{aligned} KG(P) &= 4\sqrt{2}(2h - r + 4) + (\sqrt{13} + 3\sqrt{2})(2r) + 10(6h - r - 6) \\ &= (60 + 8\sqrt{2})\,h + (2\sqrt{13} + 2\sqrt{2} - 10)\,r - (60 - 16\sqrt{2}) \\ &= 71.314h + 0.040r - 37.373 \end{aligned}$$

Note that the r-dependence of both Sombor indices is same for benzenoids and phenylenes.

4. Conclusion

In this study, the Sombor and KG-Sombor indices of benzenoid systems and phenylenes are determined. The formulas deduced make it possible to easily calculate the *SO*- and *KG*-indices for any benzenoid and phenylene graph. In both cases, these depend (in a linearly increasing manner) on the number of vertices, number of hexagons, and number of inlets. The KG-Sombor index is always greater than the Sombor index. In particular, for any benzenoid system B, $KG(B) > 2SO(B)$.

By comparing Eqs. (3) and (4), it is evident why *KG* has the name "Sombor". The prefix *KG* was added to this name, what may be understood as an abbreviated form of *Kulli-Gutman.*

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Conflict of interest. The authors declare that they have no conflict of interest.

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