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Short Communication

ON EULER-SOMBOR INDEX OF BENZENOIDS AND PHENYLENES

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ABSTRACT. The Euler-Sombor index of a graph, *EU(G)*, is a recently introduced vertex-degree based topological index. It is derived from the geometric consideration of a graph. In this paper, we provide general formulae for the computation of *EU(G)*, for a molecular graph representing a benzenoid or phenylene system.

Keywords: graph invariant, molecular structure descriptor, topological index, degree of a vertex.

Let *G* be a simple undirected graph with *n* vertices and *m* edges. Its vertex and edge sets are *V(G)* and *E(G)*, respectively. With d_u we denote the degree of a vertex *u*. If the vertices *u* and *v* are adjacent, then the edge connecting them is denoted by *uv*. For other graph-theoretical notions and definitions, the readers are referred to textbooks (BONDY and MURTY, 1976; TRUDEAU, 1993). Graph indices have found special use beyond graph theory, especially in chemistry (TODESCHINI and CONSONNI, 2009). Sometimes they are referred to as topological indices (*TIs*). In the current graph theory, there are dozens of graph indices based on the degree of a vertex (GUTMAN, 2013). Many of them are of the form (VUKIČEVIĆ and GAŠPEROV, 2010):

$$TI(G) = \sum_{uv \in E(G)} F(d_u, d_v) \tag{1}$$

where the summation of the function $F(d_u,d_v)$ goes over all edges of a graph. It is worth noting that function $F(d_u,d_v)$ satisfies the condition $F(x,y) = F(y,x)$.

Let $m_{i,j}$ denote the number of edges connecting vertices of degree *i* and degree *j*, then Eq. 1 can be written as:

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

Recently, a novel geometric approach to vertex-degree-based graph indices has been introduced (GUTMAN, 2021). Even though it was recently defined, the so-called Sombor index of a graph, *SO(G)*, gained huge attention from researchers, and many studies have been

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published (Cruz *et al.*, 2021; Das *et al.*, 2021; Redžepović, 2021; Du *et al.*, 2024; Rada *et al.*, 2024). Therefore, its properties now are relatively well understood. The Sombor index of a graph is defined as (Gutman, 2021):

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}. \quad (3)$$

A novel vertex-degree-based topological index derived from the geometric consideration of a graph is the Euler-Sombor index *EU(G)*, and it is defined as (Tang *et al.*, 2024):

$$EU(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2 + d_u d_v}. \quad (4)$$

For more details on *EU(G)*, the readers may find in recent papers (Gutman, 2024; Hu *et al.*, 2024; Gutman *et al.*, 2025). In this paper, we are concerned with the benzenoid and phenylene molecular graphs. Namely, we provide general formulae for the computation of *EU(G)* of these graphs by simply counting its structural details. The results on *SO(G)* have been published in a recent study (Kulli and Gutman, 2022).

The benzenoid and phenylene compounds are of high interest in chemistry, material science, and environmental protection. Molecular graphs derived from these molecules are depicted in Fig 1.

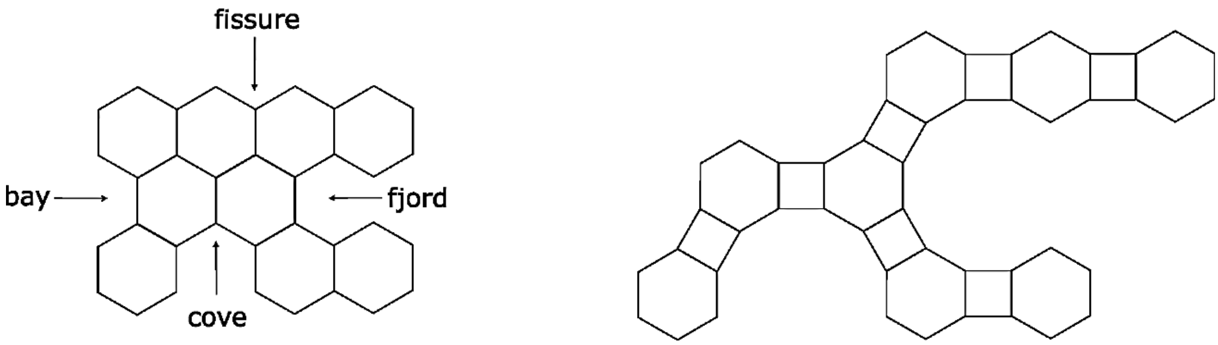

Figure 1. Left: A benzenoid graph *B* and structural features on its perimeter. In this case, *B* has four fissures, one bay, one cove, and one fjord. Thus, its number of inlets is $r = 4+1+1+1 = 7$. Right: A phenylene graph *PH*.

As one may see, these graphs contain only vertices of degree 2 and degree 3. Therefore, all their edges are of type (2,2), (2,3), and (3,3). Consequently, Eq. 2 in case of these graphs has the simple following form:

$$EU(B) = EU(PH) = F(2,2)m_{2,2} + F(2,3)m_{2,3} + F(3,3)m_{3,3}. \quad (5)$$

The values of *F(2,2)*, *F(2,3)*, and *F(3,3)* follow immediately from Eq. 4:

$$F(2,2) = 2\sqrt{3}$$
$$F(2,3) = \sqrt{19}$$
$$F(3,3) = 3\sqrt{3}$$

The dependence of physicochemical properties of benzenoids and phenylenes on structural details is a highly investigated topic. Thus, the main topological features are determined by three parameters:

n – number of vertices; h – number of hexagons; and r – number of inlets.

The number of inlets represents the number of structural details on the perimeter, see Fig. 1. The number of edges of the type (2,2), (2,3), and (3,3) in a benzenoid graph B with n vertices, h hexagons, and r inlets is (GUTMAN and CYVIN, 1989; GUTMAN, 1992):

$$m_{2,2} = n - 2h - r + 2 \tag{6}$$

$$m_{2,3} = 2r \tag{7}$$

$$m_{3,3} = 3h - r - 3. \tag{8}$$

Let n_i be the number of internal vertices of B, then (GUTMAN and CYVIN, 1989):

$$n = 4h + 2 - n_i. \tag{9}$$

By incorporating Eqs. 6–9 in Eq. 5, we get:

$$\begin{aligned} EU(B) &= F(2,2)(2h - n_i - r + 4) + F(2,3)2r + F(3,3)(3h - r - 3) \\ &= 2\sqrt{3}(2h - n_i - r + 4) + 2\sqrt{19}r + 3\sqrt{3}(3h - r - 3) \\ &= 13\sqrt{3}h + \left(2\sqrt{19} - 5\sqrt{3}\right)r - \sqrt{3} - 2\sqrt{3}n_i \\ &= 22.517h + 0.058r - 1.732 - 3.464n_i \end{aligned}$$

Note that for the catacondensed benzenoid system $n_i = 0$.

The number of edges of type the (2,2), (2,3), and (3,3) in a phenylene graph PH with h hexagons and r inlets is (RADA *et al.*, 2001):

$$m_{2,2} = 2h - r + 4 \tag{10}$$

$$m_{2,3} = 2r \tag{11}$$

$$m_{3,3} = 6h - r - 6. \tag{12}$$

By incorporating Eqs. 10–12 in Eq. 5, we get:

$$\begin{aligned} EU(PH) &= F(2,2)(2h - r + 4) + F(2,3)2r + F(3,3)(6h - r - 6) \\ &= 2\sqrt{3}(2h - r + 4) + 2\sqrt{19}r + 3\sqrt{3}(6h - r - 6) \\ &= 22\sqrt{3}h + \left(2\sqrt{19} - 5\sqrt{3}\right)r - 10\sqrt{3} \\ &= 38.105h + 0.058r + 17.321 \end{aligned}$$

It is interesting to note that the dependence of r is the same, both for the benzenoid and phenylene graphs.

The Euler-Sombor index is a novel vertex-degree-based topological index, and, in this study, it is determined for benzenoids and phenylenes. These are compounds of a high interest. The presented formulae make it possible to easily calculate *EU(B)* and *EU(PH)* by simply counting the structural details for any benzenoid and phenylene graph. It was found that *EU(B)* and *EU(PH)* depend on the number of vertices n, the number of hexagons h, and the number of inlets r. It is interesting that the r-dependence is the same in both cases.

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