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A NEW METHOD FOR COMPUTING THE ECCENTRIC CONNECTIVITY INDEX OF FULLERENES

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Abstract. The eccentric connectivity index of the molecular graph G, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan. It is defined as $\xi^c(G) = \Sigma_{u\in V(G)} \deg_G(u)\,\mathrm{ecc}(u)$, where $\deg_G(x)$ denotes the degree of the vertex x in G and $\mathrm{ecc}(u) = \mathrm{Max}\{d(x,u) \mid x \in V(G)\}$. In this paper this graph invariant is computed for an infinite class of fullerenes by means of group action.

1. Introduction. Mathematical chemistry is a branch of pure chemistry for prediction of Chemical phenomena. Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place. Here, we recall some algebraic definitions that will be used in the paper. Throughout this paper, graph means simple connected graph. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. If $x, y \in V(G)$ then the distance $d(x, y)$ between x and y is defined as the length of a minimum path connecting x and y.

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Nowadays very many topological indices have been defined for various purposes. The eccentric connectivity index is one of the topological indices used for QSAR and QSPR studies. This graph invariant was proposed by Sharma, Goswami and Madan [12]. It is defined as $\xi^c(G) = \Sigma_{u\in V(G)} \deg(u)\varepsilon(u)$, where $\deg(x)$ denotes the degree of the vertex x in G and $\varepsilon(u) = \mathrm{Max}\{d(x,u) \mid x \in V(G)\}$, [1–7, 16]. The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G, respectively. Another topological index defined by Gupta, Singh and Madan [8] is connective eccentric index. This topological index was defined as

$$C^{\xi}(G) = \sum_{u\in V(G)} \frac{\deg(u)}{\varepsilon(u)}.$$

The fullerene era started in 1985 with the discovery of a stable C_{60} cluster and its interpretation as a cage structure with the familiar shape of a soccer ball, by Kroto and his co-authors [10]. The well-known fullerene, the C_{60} molecule, is a closed-cage carbon molecule with three-coordinate carbon atoms tiling the spherical or nearly spherical surface with a truncated icosahedral structure formed by 20 hexagonal and 12 pentagonal rings [11]. Let p, h, n and m be the number of pentagons, hexagons, carbon atoms and bonds between them in a given fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = (5p + 6h)/3$, the number of edges is $m = (5p + 6h)/2 = 3/2n$ and the number of faces is $f = p + h$. By Euler's formula $n - m + f = 2$, one can deduce that $(5p + 6h)/3 - (5p + 6h)/2 + p + h = 2$, and therefore $p = 12$, $v = 2h + 20$ and $e = 3h + 30$. This implies that such molecules are made up entirely of n carbon atoms and have 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20. Herein, our notation is standard and taken from the standard book of graph theory [9].

2. Results and discussion. The aim of this section is to compute the eccentric connectivity index and then the connective eccentric index of an infinite family of fullerenes as depicted in Figure 1.

Before going on to calculate this index for fullerene graphs, we must compute the eccentric connectivity index for some well-known class of graphs:

Example 1. Consider the fullerene graph C_{20} (Figure 2). One can see that for every $x \in V(G)$, $\mathrm{ecc}(x) = 5$. This implies that

$$\xi^C(G) = \sum_{a\in V(G)} 3 \times 5 = 300, \text{ and so, } C^{\xi}(G) = \sum_{a\in V(G)} \frac{3}{5} = 12.$$

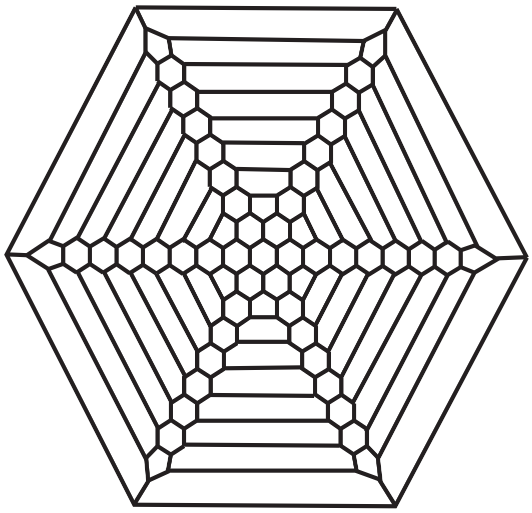

Fig. 1. 2-D graph of fullerene C_{24n}, for $n = 8$

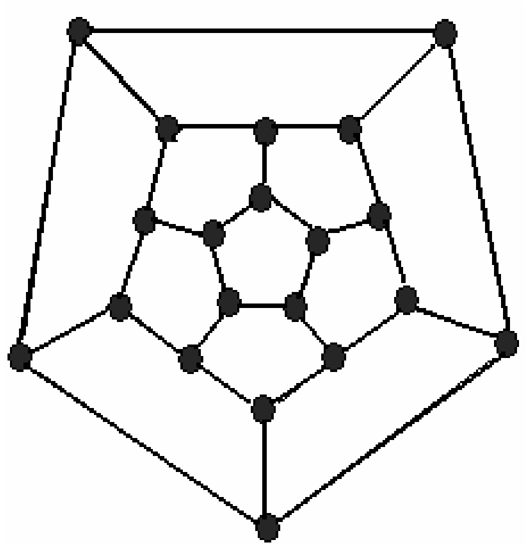

Fig. 2. 2-D graph of fullerene C_{20}

Generally, it is easy to see that for every k-regular graph we have:

$$\xi^C(G) = k \sum_{a \in V(G)} \mathrm{ecc}(a) \quad \text{and} \quad C^\xi(G) = k \sum_{a \in V(G)} \mathrm{ecc}(a)^{-1}.$$

Example 2. Suppose K_n denotes the complete graph on $n$vertices. Then for every vertex $v \in V(K_n)$, $\deg(v) = n - 1$ and $\mathrm{ecc}(v) = 1$. So, $\xi^C(G) = C^\xi(G)(n-1)\sum_{a \in V(G)} 1 = n(n-1)$.

2.1. Symmetry group. Symmetry plays a central role in the analysis of the structure, bonding, and spectroscopy of molecules. Chemists classify molecules according to their symmetry. The collection of symmetry elements present in a molecule forms a group, typically called a point group. Since all the symmetry elements (points, lines, and planes) will intersect at a single point, we name it point group. The symmetry properties of objects (and molecules) may be described in terms of the presence of certain symmetry elements and their associated symmetry operations. Symmetry elements are properties which are related to the structure of the molecule. They include mirror planes, axes of rotation, centers of inversion and improper axes of rotation. (An improper axis of rotation is a rotation followed by a reflection perpendicular to the rotational axis.) Symmetry operations are actions which place the molecule in an orientation which appears to be identical to its initial orientation. Symmetry operations include rotation, reflection, inversion, rotation followed by reflection, and identity. The identity operation simply leaves the molecule where it is. All molecules have the identity operation. Certain physical properties of molecules are clearly linked to molecular symmetry. Molecules which are symmetrically bonded to the same elements will not be polar, due to the canceling dipole moments. Likewise, chirality (left or right handedness) is clearly a symmetry property. Chirality can only be present in molecules which lack an improper axis or rotation. Molecules with a center of inversion or a mirror plane cannot be chiral. The symmetry properties of molecules are tabulated on character tables. A character table lists the symmetry elements of the point group, along with characters which are consistent with the different symmetry operations of the group. The table characterizes how various atomic properties (the symmetry of atomic orbitals, rotations about axes, etc) are transformed by the symmetry operations of the group.

In this section we compute the symmetry group of fullerenes C_{24n}. The generators of its symmetry group will be indicated by a and b, whereas a stands for a reflection. In the first step, consider the labeling of vertices of the fullerene C_{72} as is indicated in Figure 3: the permutation representation of generators of the symmetry group acting on the set of vertices is given by $a := (1, 28, 31, 54, 43, 64,$

$50, 56, 39, 30, 13, 25)(2, 24, 10, 44, 51, 70, 59, 65, 49, 37, 16, 21)(3, 9, 32, 52, 60, 69, 68, 66, 48, 27, 19, 17)(4, 23, 42, 61, 62, 72, 67, 57, 38, 22, 14, 8)(5, 34, 41, 63, 53, 71, 58, 47, 20, 26, 7, 18)(6, 35, 11, 45, 33, 55, 40, 46, 15, 36, 12, 29)$;
$b := (1, 25)(2, 18)(3, 8)(4, 17)(5, 21)(6, 29)(7, 24)(9, 14)(10, 26)(11, 36)(12, 35)(13, 28)(15, 45)(16, 34)(19, 23)(20, 44)(22, 32)(27, 42)(30, 31)(33, 46)(37, 41)(38, 52)(39, 54)(40, 55)(43, 56)(47, 51)(48, 61)(49, 63)(50, 64)(53, 65)(57, 60)(58, 70)(59, 71)(62, 66)(67, 69)(68, 72)$.

The generators satisfy in the following relations:

$$a^{12} = b^2 = 1 \text{ and } bab = a^{11} = a^{-1}.$$

This implies that the symmetry group of fullerene C_{72} is isomorphic with the Dihedral group D_{24}. By using GAP [14], one can see that the symmetry group S of C_{24n} fullerene is isomorphic to the Dihedral group D_{24} of order 24 and the cycle types of elements of S are as in Table 1. By the above discussion we have proven the following Theorem:

Theorem 3. *The symmetry group of the fullerene graph C_{24n} ($n \geq 3$) is isomorphic with Dihedral group D_{24}.*

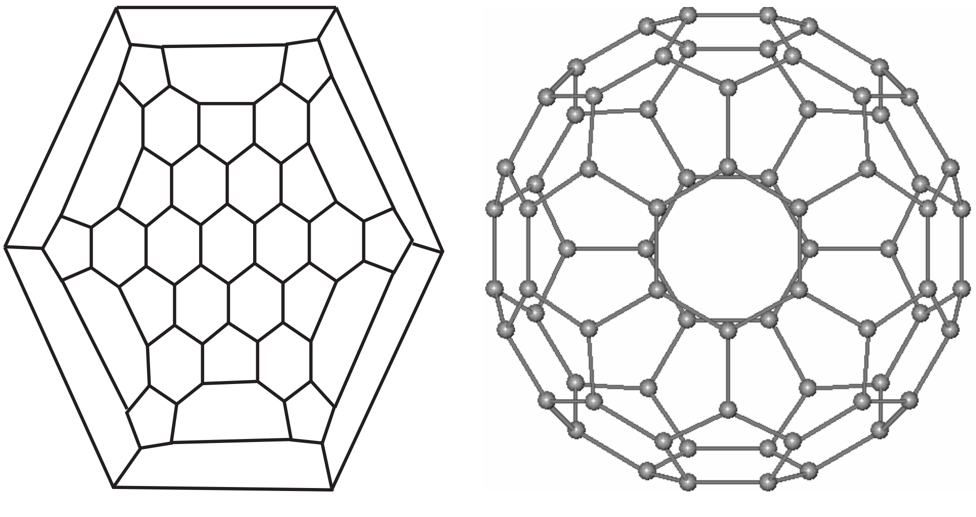

Fig. 3. 2-D and 3-D graph of fullerene C_{24n}, for $n = 3$

2.2. Vertex-transitive graphs. As we know groups are often used to describe symmetries of objects. This is formalized by the notion of group action. Let G be a group and X a nonempty set. An action of G on X is denoted by

Table 1. Cycle type of elements of symmetry group of fullerene C_{24n}

#Permutations	Cycle type	Fullerene
1	1^{24n}	
6	$1^4 2^{12n-2}$	
7	2^{12n}	
2	3^{8n}	C_{24n}
2	4^{6n}	
2	6^{4n}	
4	12^{2n}	

GX and X is called a G-set. It induces a group homomorphism φ from G into the symmetric group S_X on X, where $\varphi(g)x = gx$ for all $x \in X$. The orbit of x will be denoted as x^G and defines as the set of all $\varphi(g)x$, $g \in G$.

A bijection σ on vertices set of graph G is named an automorphism of the graph if it preserves the edge set. In other words, σ is an automorphism if $e = uv$ is an edge, then $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E. Let $Aut(G) = \{\alpha : V \to V, \alpha \text{ is bijection}\}$, then $Aut(G)$ under the composition of mappings forms a group. We say that $Aut(G)$ acts transitively on V if for any vertices u and v in V there is $\alpha \in Aut(G)$ such that $\alpha(u) = v$. Similarly, the edge transitive graph can be defined.

Lemma 4 ([2]). *Suppose G is a graph, $A_1, A_2, \ldots, A_t$ are the orbits of $Aut(G)$ under its natural action on $V(G)$ and $x, y \in A_i$, $1 \le i \le t$. Then* $\mathrm{ecc}(x) = \mathrm{ecc}(y)$. *In particular, if G is vertex transitive then for every pair (u, v) of vertices* $\mathrm{ecc}(u) = \mathrm{ecc}(v)$.

Now we are ready to compute the eccentric connectivity index of fullerene C_{24n}. To do this, first consider some exceptional cases ($3 \le n \le 6$) for this class of fullerenes:

$$\begin{aligned}\xi(C_{72}) &= 3 \sum_{u \in C_{72}} \varepsilon(u) \\ &= 3(48 \times 17 + 24 \times 16 + 24 \times 15 + 24 \times 14 + 24 \times 13 + 24 \times 12) \\ &= 7488.\end{aligned}$$

$$\xi(C_{96}) = 3 \sum_{u \in C_{96}} \varepsilon(u)$$

$$= 3(48 \times 17 + 24 \times 16 + 24 \times 15 + 24 \times 14 + 24 \times 13 + 24 \times 12)$$
$$= 7488.$$

$$\xi(C_{120}) = 3 \sum_{u \in C_{120}} \varepsilon(u)$$
$$= 3(48 \times 17 + 24 \times 16 + 24 \times 15 + 24 \times 14 + 24 \times 13 + 24 \times 12)$$
$$= 7488.$$

$$\xi(C_{144}) = 3 \sum_{u \in C_{144}} \varepsilon(u)$$
$$= 3(48 \times 17 + 24 \times 16 + 24 \times 15 + 24 \times 14 + 24 \times 13 + 24 \times 12)$$
$$= 7488.$$

For $n \geq 7$ we can prove the following Theorem:

Theorem 5. $\xi^C(C_{24n}) = 108n^2 + 324n - 72$*and* $C^{\xi}(C_{24n}) = 108n^2 + 324n - 72$.

Proof. By using GAP software one can see that the number of orbits of group D_{24} on the set $\{1, 2, \ldots, 24n\}$ can be divided into 2 classes, namely $[u]$ and $[v]$. To reach vertex x from vertex u, we must pass through n hexagons and one pentagon, see Figure 4. This implies that the eccentricity of vertex u is $2n + 3$. Obviously, the eccentricity of other vertices is as shown in Table 2.

Table 2. The eccentricity of vertices in C_{24n} fullerene

Vertices	Ecc(x)	No
The type 1 vertices	$2n + 3$	48
The type 2 vertices	$2n + 3 - i$, $1 \leq i \leq n - 2$	24

By using the values reported in this table the eccentric connectivity index is as follows:

$$\xi^C(C_{24n}) = \sum_{u \in C_{24n}} \varepsilon(u)\deg(u) = 3 \sum_{u \in F_{24n}} \varepsilon(u)$$
$$= 3(48(2n + 3) + 24(2n + 2) + 24(2n + 1) + \cdots + 24(n + 5))$$

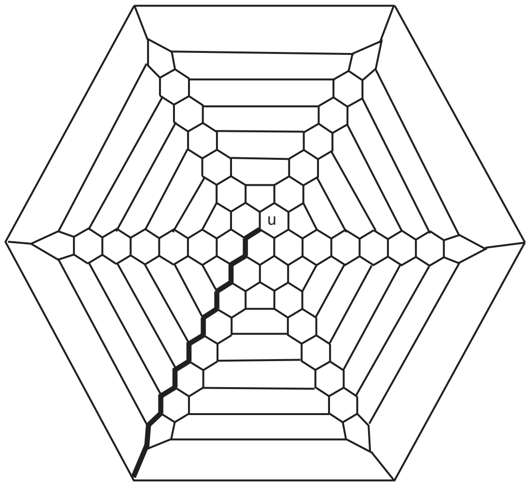

Fig. 4. The eccentricity of vertex u

$$= 72\left(\frac{n-1}{2}[2n+10+n-2]+(2n+3)\right)$$

$$= 36(n-1)(3n+8)+(144n+216)$$

$$= 108n^2+324n-72.$$

By using these calculations and Figure 4, the theorem is proved.

Corollary 6. *The connective eccentric index of* C_{24n} *is as follows:*

$$C^{\xi}(C_{24n}) = \sum_{u\in C_{24n}} \deg(u)\varepsilon(u)^{-1}$$
$$= 3(48/(2n+3)+24/(2n+2)+24/(2n+1)+\cdots+24/(n+5)).$$

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