# A note on k-regular edge connectivity of fullerenes

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**Abstract:** Fullerenes are polycyclic molecules have broad applications from the chemistry, pharmacology to physics and electronic sciences. M-barrel fullerenes are a generalized class of fullerenes. Connectivity concept in chemical graph theory gives information about underlying topology of chemical structures, fault tolerance of molecules and vulnerability of chemical networks. In this study we computed k-regular edge connectivity, almost k-regular connectivity for m-barrel fullerenes. This calculation gives information about fault tolerance for m-barrel fullerenes.

**Keywords:** connectivity, fullerene, k-regular edge connectivity, almost k-regular connectivity, m-barrel fullerene

## 1 Introduction

Fullerenes are equivalent to carbon sphere-shaped substances in chemistry which they consist of the basis for thousands of patents for a wide range of applications from chemistry to electronic, physical and medical sciences (Planeix et al., 1994; Da Ross and Prato, 1999). QSPR/QSAR researches involve graph theoretical analysis of chemical substances. These investigations enable to predict physical and chemical properties of chemical substances without conducting very expensive experimental studies. These studies also give the knowledge of underlying topology of molecules. There are many studies about mathematical especially graph theoretical approaches to analyse fullerenes. Fullerenes and coordination polyhedral versus half-cube embeddings were investigated in (Deza et al., 1998). Four-dimensional football, fullerene and diagram geometry was studied in (Pasini, 2001). Constructing fullerene graphs from their eigenvalues and angles was initated in (Cevetković et al., 2002). Encoding fullerenes and geodesic domes were analysed in (Graver, 2004). Spectral moments of fullerene graphs were studied in (Cvetković and Števanović, 2004). The independence numbers of fullerenes and benzenoids were investigated in (Graver, 2006). The smallest eigenvalue of fullerene graphs-closing the gap was calculated in (Došlić, 2013).

The fault–tolerance of a chemical network is an important measure to conduct reliable studies in view of chemical information and modelling. Connectivity notion in graph theory is one of the leading means determining fault-tolerance of chemical networks. But classical connectivity is not enough to determine fault-tolerance and vulnerability of chemical networks since it assumes every atom has equivalent role in chemical point of view. To handle this problem, Harary posed conditional connectivity notion in graph theory (Harary, 1983). After that, many conditional connectivity measures were defined in the literature such as; cycle-edge connectivity, restricted connectivity, extra connectivity, structure connectivity. Restricted connectivity was defined in (Esfahanian and Hakimi,1988). Extra connectivity was initiated in (Fabrega and Fiol, 1996). Super-connectivity and super-edge-connectivity for some interconnection networks were investigated in (Chen et al, 2003). Restricted h-connectivity measures for large multiprocessor systems were studied in (Latifi et al., 1994). Structure connectivity and substructure connectivity of hypercubes were defined in (Lin et al., 2016). On the cyclic connectivity of planar graphs were firstly studied independently from conditional connectivity in (Plummer, 1972). Two novel conditional connectivity based on regularity have been defined by the present authors: k-regular edge connectivity and almost k-regular edge connectivity (Ediz and Çiftçi, 2022).

Cycle-edge connectivity measurement for fullerenes was initiated in (Došlić, 2003). Restricted edge connectivity and cycle-edge connectivity of m-barrel fullerenes which they are a generalization of classical fullerenes, have been investigated very recently (Tarakmi et al., 2021).

As a continuation of these similar studies, we computed k-regular edge connectivity and almost k-regular edge connectivity notions for m-barrel fullerene graphs.

## 2 Materials and Method

Necessary definitions are given in order to prepare the reader for calculations of the k-regular edge connectivity and almost k-regular connectivity.

Let $G=(V,E)$ a connected graph where $V$ is the vertex set and $E$ is the edge set. The degree of any vertex(atom, node) of $G$ is the number of edges(bond, link) incident to this vertex and denoted as, deg $v$ for the vertex $v$ of $V$. If all the degrees of the vertices of $G$ equal $r$, then $G$ is called $r$-regular graph. A 3-regular graph is named as cubic graph. Notice that fullerenes are 3-regular and therefore they are cubic graphs. 2-regular connected graphs with n-edge and n-vertex are called cycles and denoted as $C_n$. If an edge deleted from the cycle $C_n$ then the path graph $P_n$ is acquired. If an n-vertex graph, every vertex is adjacent to the other all vertices then this graph is called complete graph and denoted as $K_n$. Connected three regular graph with all faces are pentagons and hexagons is called fullerene in respect to graph theoretical approach definition. A generalized fullerene graphs; m-barrel fullerenes defined as: A cubic graph $F(m,k)$ is called a m-barrel fullerene graph when the following conditions hold for positive integers $m \geq 3$ and $k \geq 1$,

i) $F(m,k)$ consists of $k+3$ concentric circles with each circle has $2m$ vertices except from the first (the innermost) and the last (the outermost) circles,

ii) The first and the last circles are represented as an $m$-gon,

iii) $F(m,k)$ has $k+2$ layers,

iv) The first and the last layers are represented as $m$ number of m-gons and the other $k$ layers are represented as $m$ number of hexagons.

Edge connectivity of a connected graph $G$, $\lambda(G)$, is the minimum number of edges whose deletion make the graph $G$ disconnected.

And now we give the definitions of two novel conditional connectivity measures: k-regular edge connectivity and almost k-regular edge connectivity (Ediz and Çiftçi, 2022). Let $G$ be a graph and $S$ be a set of edges. If $G$-$S$ is disconnected and each component is a k-regular graph then $S$ is called a k-regular edge cut of $G$. The minimum cardinality of a k-regular edge cut of $G$ is called k-regular edge connectivity of $G$ and denoted as; $\lambda^{kr}(G)$ (Ediz and Çiftçi, 2022).

Similar definition can be given as for almost k-regular connectivity of $G$. Let $G$ be a graph and $S$ be a set of edges. If $G$-$S$ is disconnected and $|\deg u - \deg v| \leq k$ for any two vertices belong to any disconnected component then $S$ is called an almost k-regular edge cut of $G$. The minimum cardinality of an almost k-regular edge cut of $G$ is called almost k-regular edge connectivity of $G$ and denoted as; $\lambda^{akr}(G)$ (Ediz and Çiftçi, 2022).

And now, we begin to compute the k-regular edge connectivity and almost k-regular edge connectivity for m-barrel fullerenes. We use combinatorial computing techniques method in our computations.

**3 Results**

The following observations are direct consequences of definition of k-regular edge connectivity notion.

Observation 1. (Ediz and Çiftçi, 2002) $\lambda^{1r}(C_n) = \frac{n}{2}$ for any even number for $n \geq 4$.

Observation 2. (Ediz and Çiftçi, 2002) $\lambda^{1r}(K_n) = \frac{n(n-2)}{2}$ for any even number for $n \geq 4$.

Observation 3. (Ediz and Çiftçi, 2002) $\lambda^{2r}(K_n) = \frac{n(n-3)}{2}$ for any integer for $n \geq 4$.

Observation 4. (Ediz and Çiftçi, 2002) $\lambda^{3r}(K_n) = \frac{n(n-4)}{2}$ for any even number for $n \geq 8$.

Observation 5. (Ediz and Çiftçi, 2002) $\lambda^{4r}(K_n) = \frac{n(n-5)}{2}$ for any integer for $n \geq 10$.

Theorem 6. (Ediz and Çiftçi, 2002) $\lambda^{kr}(K_n) = \frac{n(n-k-1)}{2}$ for suitable integers $n$ and $k$.

The following propositions are related to compute 2-regular and 1-regular edge connectivity for m-barrel fullerenes *F(m,k)*.

Theorem 7. $\lambda^{2r}(F(m,k)) = km + 2m$.

Proof. We know from the definition of 2-regular edge connectivity that we must to disconnect $F(m,k)$ into disconnected components such that all of them are 2-regular graphs that is cycles. It is known that $F(m,k)$ has $k+2$ layers from the definition of m-barrel fullerenes and Fig. 1. Each layer has $m$ number of edges incident to neighbouring layer. Therefore, deletion of these $m$ number of edges within each layer gives $k+2$ disconnected nested cycles. Thus, $\lambda^{2r}(F(m,k)) = m(k+2) = km + 2m$.

Theorem 8. $\lambda^{1r}(F(m,k)) = 2km + 4m$ for even integer $m \geq 4$.

Proof. We know from the definition of 1-regular edge connectivity that we must to disconnect $F(m,k)$ into disconnected components such that all of them are 1-regular graphs that is $K_2$. It is shown that $\lambda^{2r}(F(m,k)) = m(k+2) = km + 2m$ in Theorem 7. We will continue the proof through the rest of disconnected cycles in the proof of Theorem 7. It is necessary to delete of minimum number of suitable edges in each $k+3$ concentric cycles. The innermost and the outermost cycles are isomorphic to $C_m$. Remaining $k+1$ cycles are isomorphic to $C_{2m}$. With the help of Observation 1, $\lambda^{1r}(C_m) = \frac{m}{2}$ and $\lambda^{1r}(C_{2m}) = m$ can be written. Therefore, we get 1-regular edge connectivity of *F(m,k)* via deletion of suitable $2\frac{m}{2} + (k+1)m$ edges in disconnected cycles in the proof of Theorem 7. Thus;

$\lambda^{1r}(F(m,k)) = km + 2m + m + km + m = 2km + 4m$. The proof is completed.

And now, we begin to calculate almost k-regular connectivity for m-barrel fullerenes.

Observation 8. (Ediz and Çiftçi, 2002) $\lambda^{a1r}(C_n) = 2$.

Proposition 9. (Ediz and Çiftçi, 2002) $\lambda^{a1r}(K_n) = 2n - 4$.

Corollary 10. $\lambda^{akr}(K_n) = 2n - 4$ for $n \geq 7$ and $1 \leq k \leq n - 1$.

And we give our last two result for the computations of almost 1-regular and almost 2-regular connectivity of m-barrel fullerenes.

Theorem 11. $\lambda^{a1r}(F(m, k)) = 4$.

Proof. We want to disconnect $F(m, k)$ into at least two disconnected graphs by deleting minimum number of edges such that the difference of any two vertices degrees equal to one or zero in every component graph. Therefore, one of the disconnected component graph must be $K_2$. Without loss of generality, we choose $K_2$ as any edge *uv* of $F(m, k)$. Deletion of four different neighbouring edges of *uv* gives the desired result.

Corollary 12. $\lambda^{a2r}(F(m, k)) = 4$.

Proof. The proof is the same as in the proof of Theorem 11.

## 4 Conclusions

The main focus of this study is to calculate k-regular edge connectivity and almost k-regular connectivity for m-barrel fullerenes. This calculation for m-barrel fullerenes is essential for understanding fault tolerance and vulnerability parameters in generalized fullerenes.

**Acknowledgement**

We thank the anonymous reviewers for their careful reading of our manuscript and their many insightful comments and suggestions.

**Research funding**

The authors state no funding involved.

**Author contribution**

**İdris Çiftçi:** Writing – original draft, Writing – review & editing, Methodology, Formal Analysis; **Süleyman Ediz:** Formal Analysis, Visualization, Project administration.

**Conflict of interest**

The authors state no conflict of interest.

**Data availability statement**

All data generated or analyzed during this study are included in this published article.

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