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Innovative Multiplicative Connectivity of Poly-ether Ketone, Poly-ether Ketone Ketone, and Poly-ether Ether Ketone

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Abstract:
Organic chemistry constantly pushes the boundaries by synthesizing new molecules each year. However, before these compounds can be practically used, rigorous testing is needed to understand their characteristics. This process can be expensive and time-consuming, requiring specialized laboratory equipment, chemicals, and personnel. To address these challenges, mathematical models are increasingly used to predict the properties of compounds theoretically. In this study, we focus on polyether ketones (PEKs), calculating their atom bond connectivity (ABC) and examining their sum-connectivity and multiplicative-connectivity indexes. Our results show that PEKs exhibit notably high atom bond connectivity, which could have promising implications for their use in material science and other advanced applications.

Keywords: Connectivity index; Polyether ketones; Randic index; Modeling properties; Mathematical Model.

1. Intorduction

The upsurge of the application of graph-theoretical structural descriptors symbolizes the heightened mathematics incorporation into contemporary chemistry, hence, an immense leap in the predictive models development path. The topological indices are a key element in this field of study. They are the only ones that remain constant even when a graph is transformed into an isomorphic version. Most of the interest in the topological indices comes from their application in QSPR (Quantitative Structure-Property Relationships) and QSAR (Quantitative Structure-Activity Relationships), which are used for measuring and analyzing the correlation between two sets of data [1,2].

One of the earliest and most widely adopted graph invariants is the connectivity index, whose introduction by Randic in 1975 is the most popular example [3]. At first, this index was established to study the branching ways of the carbon atom skeletons of alkenes. Nevertheless, its usefulness has grown, and it has been discovered that it has strong correlations with a great number of physicochemical and pharmacological properties across a big spectrum of organic compounds [4,5]. The newer member in the group of graph-theoretical invariants is "Atom-Bond Connectivity Index" that deals with the interconnection between atoms and bonds in a molecule [6.7]. The index is similar to the former one but its formulation is based on the degrees of vertices and edges rather than the branching of the molecular structures.

To explain this more formally, consider a finite, simple, connected graph where ν represents the vertices and E denotes the edges. The degree of a vertex, which is often symbolized by d for the case where d is the number of edges connected to that vertex [8]. In the context of mathematical modeling, a molecular or chemical graph is an abstract depiction of a chemical compound's structure. The vertices in this graph correspond to the atoms in the molecule, while the edges represent the bonds or links between those atoms. Topological descriptors derived from the graph are useful in determining the relationship between the structure and physicochemical properties of a compound [9].

Building on this concept, Kulli and colleagues introduced the atom bond sum connectivity index of a graph G, which further refines how these molecular connections are quantified [10].

$$ABS(\Phi) = \sum_{\mathcal{E}\nu \in E(\Phi)} \sqrt{\frac{d(\mathcal{E}) + d(\nu) - 2}{d(\mathcal{E}) + d(\nu)}}$$

We further define the multiplicative atom bond sum connectivity index as [11]

$$ABSII(\Phi) = \prod_{\mathcal{E}\nu \in E(\Phi)} \sqrt{\frac{d(\mathcal{E}) + d(\nu) - 2}{d(\mathcal{E}) + d(\nu)}}$$

The Atom-Bond Connectivity (ABC) index has, however, been documented to work well on several pillars particularly the estimation of heat of formation in organic compounds [12]. Furtula et al. also increased the scope of the ABC index by using it in the analysis of the stability of alkanes and cycloalkanes' strain energy. Their studies additionally focused on the algebraic properties of the ABC indices defined on trees which guided them in locating chemical trees that corresponded to extremes of the ABC values [13]. In another important report, Estrada et al.

managed to employ the ABC index for the heat of formation modeling of alkenes resulting in the creation of a strong QSPR (Quantitative Structure-Property Relationship) model for alkanes. In particular, the intercept and the slope of their regression equation have been quantitatively meaningful, which added confidence to the model [14].

Earlier, Kulli and his collaborators made valuable additions to this field by suggesting a number of multiplicative connectivity indices of graph-type chemical structures. These indices were used to model more complicated structures like nanotubes covered by C5 and C7 molecules [15]. In another paper by the same group out of many which presented enhanced versions of the second- and fourth-order atom-bond connectivity indices, the authors improve understanding of structures like nanotube and nanotorus for the paraffin coating around nanostructures [16].

Wei and former colleagues were also interested in the properties of a variety of nanostructures, but from a mathematical perspective. In particular, they were interested in such key nanomaterials as nanotubes, nanostars, dendrimers, and nanotori. By means of edge set-correlation using trick-type multiplicative atom-bond connectivity indices, the authors undertook work which has defined the theoretical bases that have bearing on nanoengineering [17]. Similar investigations into the atom-bond connectivity indices have been involved in a number of works [18-20].

Pushed forward by these detailed investigations on the cross chemical structure and ABC index, we opted to investigate further in Polyether ketones (PEKs). In this paper, we have calculated the atom bond sum connectivity index and the multiplicative atom bond sum connectivity index of the Poly-ether Ketone (PEK), Poly-ether Ketone Ketone (PEKK) and Poly-ether Ether Ketone (PEEK). Our research presents new contributions in the knowledge of the connectivity attributes of these important materials.

2. The ABC index of PEK

PEK is a type of polymer that comprises ketone (R-CO-R) and ether (R-O-R) functionalities in its molecular structure. These can be synthesized by combining 4,4′-difluoro benzophenone with hydroquinone's potassium or sodium salts. PEK as huge heat and wear resistanc [21-22]. This highly resilient material can endure exposure to non-oxidizing acids, oils, lubricants, water vapors, hot water, and concentrated alkalis. Its versatility makes it popular in the medical, electronics, and automotive industries [23-25].

(a)

(b)

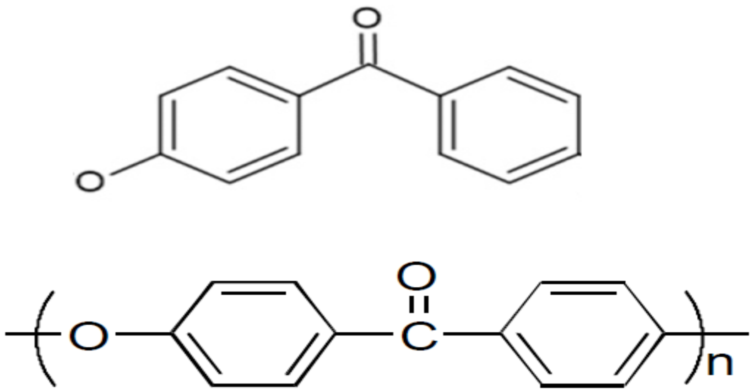

Figure 1: Abase unit of PEK (a) and PEK structure (b) for analysis .

Figure $1(a),(b)$ shows the molecular structure and unit cell of PEK.Its structure consists of total $15n$ vertices and $17n-1$ edges. We represent Polyether Ketone as K_e. We obtain that $\{d(\mathcal{E}), d(\nu) : \mathcal{E}\nu \in E(K_e)\}$ has five edge set partitions.

Table 1. Edge Partition of Polyether Ketone

$d(\mathcal{E}), d(\nu) / \mathcal{E}\nu \in E(K_e)$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Numbers of edges	1	$n-1$	$4n+2$	$10n-1$	$2n-2$

Theorem 2.1:

The atom bond sum connectivity index of Polyether Ketone

$$ABS(K_e) = \frac{1}{\sqrt{3}} + (5n+1)\frac{1}{\sqrt{2}} + (10n-1)\sqrt{\frac{3}{5}} + (2n-2)\sqrt{\frac{2}{3}}$$

Proof:

$$ABS(K_e) = \sum_{\mathcal{E}\nu \in E(K_e)} \sqrt{\frac{d(\mathcal{E}) + d(\nu) - 2}{d(\mathcal{E}) + d(\nu)}}$$

By using above definition and putting the values from Table1. We get

$$ABS(K_e) = \sqrt{\frac{1+2-2}{1+2}}(1) + \sqrt{\frac{1+3-2}{1+3}}(n-1) + \sqrt{\frac{2+2-2}{2+2}}(4n+2) + \sqrt{\frac{2+3-2}{2+3}}(10n-1) + \sqrt{\frac{3+3-2}{3+3}}(2n-2)$$

$$ABS(K_e) = \sqrt{\frac{1}{3}}(1) + \sqrt{\frac{1}{2}}(n-1) + \sqrt{\frac{1}{2}}(4n+2) + \sqrt{\frac{3}{5}}(10n-1) + \sqrt{\frac{2}{3}}(2n-2)$$

Now after some simplification we get

$$ABS(K_e) = \frac{1}{\sqrt{3}} + (5n+1)\frac{1}{\sqrt{2}} + (10n-1)\sqrt{\frac{3}{5}} + (2n-2)\sqrt{\frac{2}{3}}$$

Theorem 2.2:

The multiplicative atom bond sum connectivity index Polyether Ketone

$$ABSII(K_e) = \left(\frac{1}{3}\right)^{\frac{1}{2}} \times \left(\frac{1}{2}\right)^{\frac{5}{2}n+\frac{1}{2}} \times \left(\frac{3}{5}\right)^{5n-\frac{1}{2}} \times \left(\frac{2}{3}\right)^{n-1}$$

Proof :

By using Definition of "The multiplicative atom bond sum connectivity index"

$$ABSII(K_e) = \prod_{\mathcal{E}\nu \in E(K_e)} \sqrt{\frac{d(\mathcal{E}) + d(\nu) - 2}{d(\mathcal{E}) + d(\nu)}}$$

We get

$$ABSII(K_e) = \left(\sqrt{\frac{1+2-2}{1+2}}\right)^{1} \times \left(\sqrt{\frac{1+3-2}{1+3}}\right)^{(n-1)} \times \left(\sqrt{\frac{2+2-2}{2+2}}\right)^{(4n+2)} \times \left(\sqrt{\frac{2+3-2}{2+3}}\right)^{(10n-1)} \times \left(\sqrt{\frac{3+3-2}{3+3}}\right)^{(2n-2)}$$

$$ABSII(K_e) = \left(\frac{1}{3}\right)^{\frac{1}{2}} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(n-1)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(4n+2)} \times \left(\frac{3}{5}\right)^{\frac{1}{2}(10n-1)} \times \left(\frac{2}{3}\right)^{\frac{1}{2}(2n-2)}$$

Now some simplification will give the desired results

$$ABSII(K_e) = \left(\frac{1}{3}\right)^{\frac{1}{2}} \times \left(\frac{1}{2}\right)^{\frac{5}{2}n+\frac{1}{2}} \times \left(\frac{3}{5}\right)^{5n-\frac{1}{2}} \times \left(\frac{2}{3}\right)^{n-1}$$

3. The ABC index of PEKK

PEKK, which belongs to the poly-aryl ether ketone family, is a semi-crystalline thermoplastic that exhibits high resistance to heat, chemicals, and mechanical loads [26]. It has a variety of dental and medicinal applications. The pieces are said to be as robust as aluminum while weighing 40% less [27]. Furthermore, PEKK-produced components have demonstrated fire and radiation resistance [28].

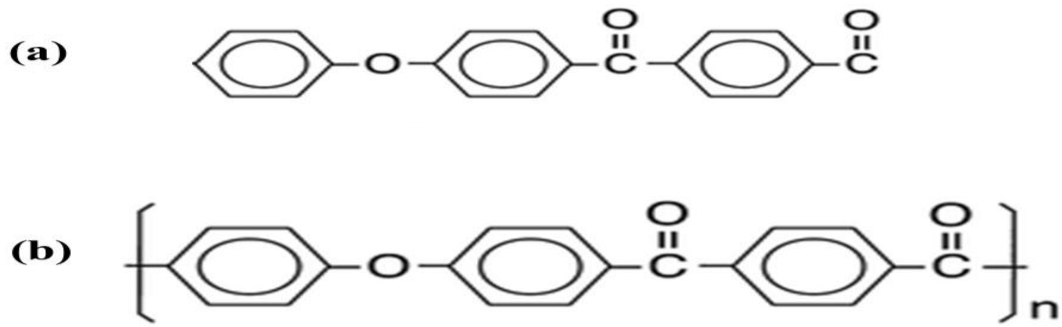

Figure 2: (a) Abase unit of PEKK (b) polymeric structure of PEKK

A unit cell of PEKK and its molecular structure is shown by Figure $2(a),(b)$. Its structure consists of total $23n$ vertices and $26n-3$ edges. We represent Polyether Ketone as E_{kk}. We obtain that $\{\mathrm{d}(\mathcal{E}),\mathrm{d}(\nu):\mathcal{E}\nu \in E(E_{kk})\}$ five edge set partitions.

Table 2: Edge Partition of PEKK

$\mathrm{d}(\boldsymbol{\mathcal{E}}),\mathrm{d}(\boldsymbol{\nu})/\ \boldsymbol{\mathcal{E}\nu} \in \boldsymbol{E(E_{kk})}$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Numbers of edges	1	$2n-1$	$6n+2$	$14n-3$	$4n-2$

Theorem 3.1:

The atom bond sum connectivity index of PEKK

$$ABS(E_{kk}) = \frac{1}{\sqrt{3}} + (8n+1)\frac{1}{\sqrt{2}} + (14n-3)\sqrt{\frac{3}{5}} + (4n-2)\sqrt{\frac{2}{3}}$$

Proof

$$ABS(E_{kk}) = \sum_{\mathcal{E}\nu\in E(E_{kk})} \sqrt{\frac{\mathrm{d}(\mathcal{E})+\mathrm{d}(\nu)-2}{\mathrm{d}(\mathcal{E})+\mathrm{d}(\nu)}}$$

By using above definition and putting the values from table 3. We get

$$ABS(E_{kk}) = \sqrt{\frac{1+2-2}{1+2}}(1) + \sqrt{\frac{1+3-2}{1+3}}(2n-1) + \sqrt{\frac{2+2-2}{2+2}}(6n+2) + \sqrt{\frac{2+3-2}{2+3}}(14n-1) + \sqrt{\frac{3+3-2}{3+3}}(4n-2)$$

$$ABS(E_{kk}) = \sqrt{\frac{1}{3}}(1) + \sqrt{\frac{1}{2}}(2n-1) + \sqrt{\frac{1}{2}}(6n+2) + \sqrt{\frac{3}{5}}(14n-1) + \sqrt{\frac{2}{3}}(4n-2)$$

Now after some simplification we get the required results

$$ABS(E_{kk}) = \frac{1}{\sqrt{3}} + (8n+1)\frac{1}{\sqrt{2}} + (14n-3)\sqrt{\frac{3}{5}} + (4n-2)\sqrt{\frac{2}{3}}$$

Theorem 3.2:

The multiplicative atom bond sum connectivity index of PEKK

$$ABSII(E_{kk}) = \left(\frac{1}{3}\right)^{1} \times \left(\frac{1}{2}\right)^{4n+\frac{1}{2}} \times \left(\frac{3}{5}\right)^{7n-\frac{3}{2}} \times \left(\frac{2}{3}\right)^{2n-1}$$

Proof:

By using Definition of "The multiplicative atom bond sum connectivity index"

$$ABSII(E_{kk}) = \prod_{\mathcal{E}\nu \in E(E_{kk})} \sqrt{\frac{d(\mathcal{E}) + d(\nu) - 2}{d(\mathcal{E}) + d(\nu)}}$$

We get

$$ABSII(E_{kk}) = \left(\sqrt{\frac{1+2-2}{1+2}}\right)^{1} \times \left(\sqrt{\frac{1+3-2}{1+3}}\right)^{(2n-1)} \times \left(\sqrt{\frac{2+2-2}{2+2}}\right)^{(6n+2)} \times \left(\sqrt{\frac{2+3-2}{2+3}}\right)^{(14n-3)} \times \left(\sqrt{\frac{3+3-2}{3+3}}\right)^{(4n-2)}$$

$$ABSII(E_{kk}) = \left(\frac{1}{3}\right)^{\frac{1}{2}} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(2n-1)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(6n+2)} \times \left(\frac{3}{5}\right)^{\frac{1}{2}(14n-3)} \times \left(\frac{2}{3}\right)^{\frac{1}{2}(4n-2)}$$

Now after some simplification will give the desired results,

$$ABSII(E_{kk}) = \left(\frac{1}{3}\right)^{1} \times \left(\frac{1}{2}\right)^{4n+\frac{1}{2}} \times \left(\frac{3}{5}\right)^{7n-\frac{3}{2}} \times \left(\frac{2}{3}\right)^{2n-1}$$

4. The ABC index of PEEK

PEEK is an organic thermoplastic polymer that is colorless and belongs to the polyaryl-ether ketone family [28]. It was prepared in November 1978 and is utilized in engineering. PEEK polymers can be made using a process known as step-growth polymerization, which is accomplished through the dialkylation of bisphenolate salts [29]. PEEK retains its high-temperature mechanical and chemical-resistance qualities [30]. It is excellent for the chemical, automotive, and aerospace industries since it is one of the few plastics that can be used in ultra-high vacuum applications.PEEK makes medical implants, such as a partial replacement skull, utilized in neurosurgery procedures [31].

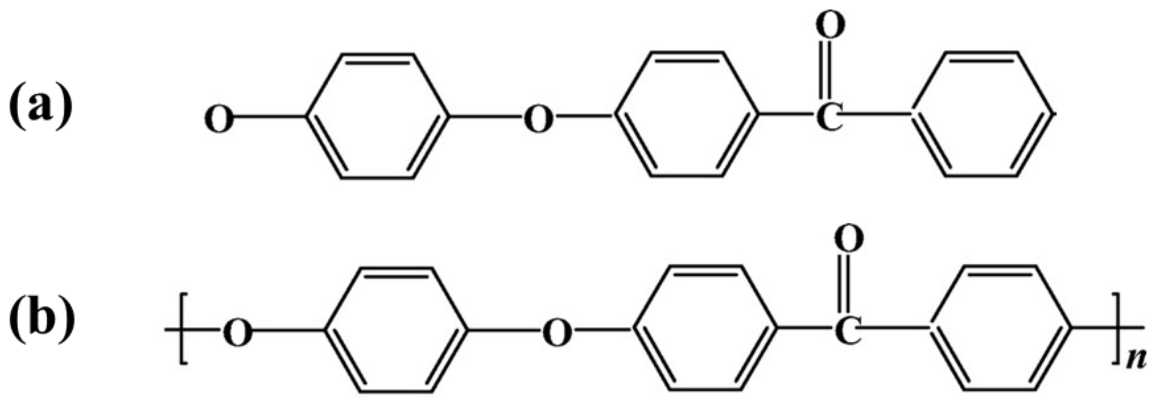

Figure 3: Abase unit of PEEK (a) Polymeric structure of PEEK (b).

A unit cell of PEEK and its molecular structure is shown by Figure $3(a),(b)$. Its structure consists of total$22n$ vertices and $25n-1$ edges. We represent PEEK as K_{ee}. We obtain that $\{ḑ(\mathcal{E}), ḑ(\nu) : \mathcal{E}\nu \in E(K_{ee})\}$ has five edge set partitions.

Table 4: Edge Partition of Poly-ether Either Ketone

$ḑ(\boldsymbol{\mathcal{E}}), ḑ(\boldsymbol{\nu}) / \boldsymbol{\mathcal{E}\nu} \in \boldsymbol{E}(\boldsymbol{K_{ee}})$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Numbers of edges	1	$n-1$	$6n+2$	$16n-1$	$2n-2$

Theorem 4.1:

The atom bond sum connectivity index of PEEK

$$ABS(K_{ee}) = \frac{1}{\sqrt{3}} + (7n+1)\frac{1}{\sqrt{2}} + (6n-1)\sqrt{\frac{3}{5}} + 2(n-1)\sqrt{\frac{2}{3}}$$

Proof:

$$ABS(K_{ee}) = \sum_{\mathcal{E}\nu \in E(K_{ee})} \sqrt{\frac{ḑ(\mathcal{E}) + ḑ(\nu) - 2}{ḑ(\mathcal{E}) + ḑ(\nu)}}$$

By using above definition and putting the values from table 3. We get

$$ABS(K_{ee}) = \sqrt{\frac{1+2-2}{1+2}}(1) + \sqrt{\frac{1+3-2}{1+3}}(n-1) + \sqrt{\frac{2+2-2}{2+2}}(6n+2) + \sqrt{\frac{2+3-2}{2+3}}(16n-1) + \sqrt{\frac{3+3-2}{3+3}}(2n-2)$$

$$ABS(K_{ee}) = \sqrt{\frac{1}{3}}(1) + \sqrt{\frac{1}{2}}(n-1) + \sqrt{\frac{1}{2}}(6n+2) + \sqrt{\frac{3}{5}}(16n-1) + \sqrt{\frac{2}{3}}(2n-2)$$

Now after some simplification we get the required results

$$ABS(K_{ee}) = \frac{1}{\sqrt{3}} + (7n+1)\frac{1}{\sqrt{2}} + (6n-1)\sqrt{\frac{3}{5}} + 2(n-1)\sqrt{\frac{2}{3}}$$

Theorem 4.2:

The multiplicative atom bond sum connectivity index of Poly-ether Either Ketone

$$ABSII(K_{ee}) = \left(\frac{1}{3}\right)^{\frac{1}{2}} \times \left(\frac{1}{2}\right)^{\frac{7}{2}n+\frac{1}{2}} \times \left(\frac{3}{5}\right)^{8n-\frac{1}{2}} \times \left(\frac{2}{3}\right)^{n-1}$$

Proof :

By using Definition of “The multiplicative atom bond sum connectivity index”

$$ABSII(K_{ee}) = \prod_{\mathcal{E}\nu \in E(K_{ee})} \sqrt{\frac{d(\mathcal{E}) + d(\nu) - 2}{d(\mathcal{E}) + d(\nu)}}$$

We get

$$ABSII(K_{ee}) = \left(\sqrt{\frac{1+2-2}{1+2}}\right)^{1} \times \left(\sqrt{\frac{1+3-2}{1+3}}\right)^{(n-1)} \times \left(\sqrt{\frac{2+2-2}{2+2}}\right)^{(6n+2)} \times \left(\sqrt{\frac{2+3-2}{2+3}}\right)^{(16n-1)} \times \left(\sqrt{\frac{3+3-2}{3+3}}\right)^{(2n-2)}$$

$$ABSII(K_{ee}) = \left(\frac{1}{3}\right)^{\frac{1}{2}} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(n-1)} \times \left(\frac{1}{2}\right)^{\frac{1}{2}(6n+2)} \times \left(\frac{3}{5}\right)^{\frac{1}{2}(16n-1)} \times \left(\frac{2}{3}\right)^{\frac{1}{2}(2n-2)}$$

Now after some simplification will give the desired results,

$$ABSII(K_{ee}) = \left(\frac{1}{3}\right)^{\frac{1}{2}} \times \left(\frac{1}{2}\right)^{\frac{7}{2}n+\frac{1}{2}} \times \left(\frac{3}{5}\right)^{8n-\frac{1}{2}} \times \left(\frac{2}{3}\right)^{n-1}$$

Table 4. The atom bond sum connectivity index for PEK, PEKK and PEEK.

n	ABS (PEK)	ABS (PEKK)	ABS (PEEK)
1	11.79136	17.09487	10.10719

2	24.70585	36.86206	21.33751
3	37.62035	56.62926	32.56783
4	50.53484	76.39645	43.79815
5	63.44934	96.16364	55.02847
6	76.36383	115.9308	66.25879
7	89.27832	135.698	77.48911
8	102.1928	155.4652	88.71943
9	115.1073	175.2324	99.94975
10	128.0218	194.9996	111.1801

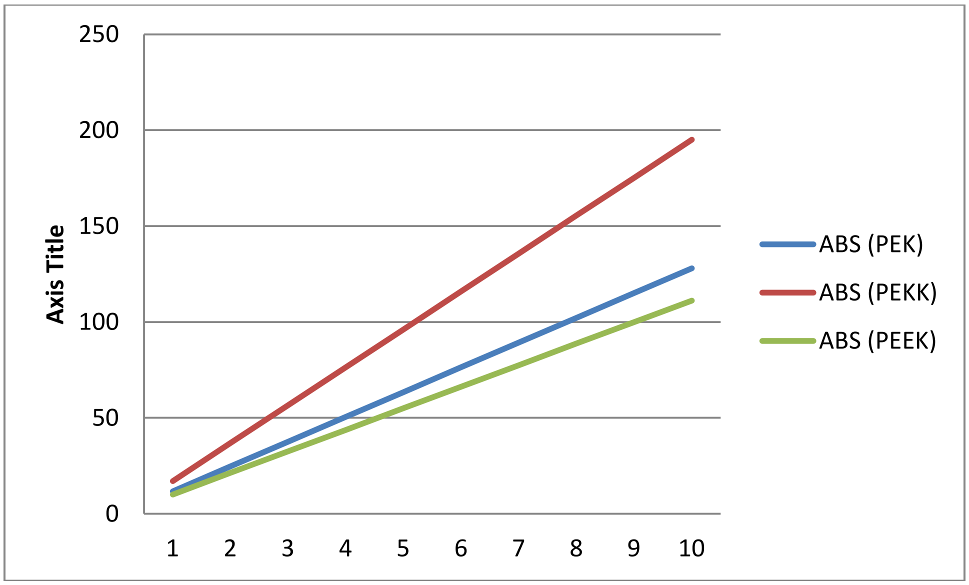

Figure 4: Comparison of atom bond sum connectivity index for PEK, PEKK and PEEK.

Table 5. The multiplicative atom bond sum connectivity index for PEK, PEKK and PEEK.

n	$ABSII(K\_ee)$	$ABSII(E\_kk)$	$ABSII(K\_e)$
1	0.000782	0.000592	0.007245
2	7.74E-07	4.60E-07	6.64E-05
3	7.66E-10	3.58E-10	6.08E-07
4	7.59E-13	2.78E-13	5.58E-09
5	7.51E-16	2.16E-16	5.11E-11
6	7.43E-19	1.68E-19	4.68E-13
7	7.35E-22	1.31E-22	4.29E-15
8	7.28E-25	1.02E-25	3.93E-17

9	7.20E-28	7.91E-29	3.60E-19
10	7.13E-31	6.15E-32	3.30E-21

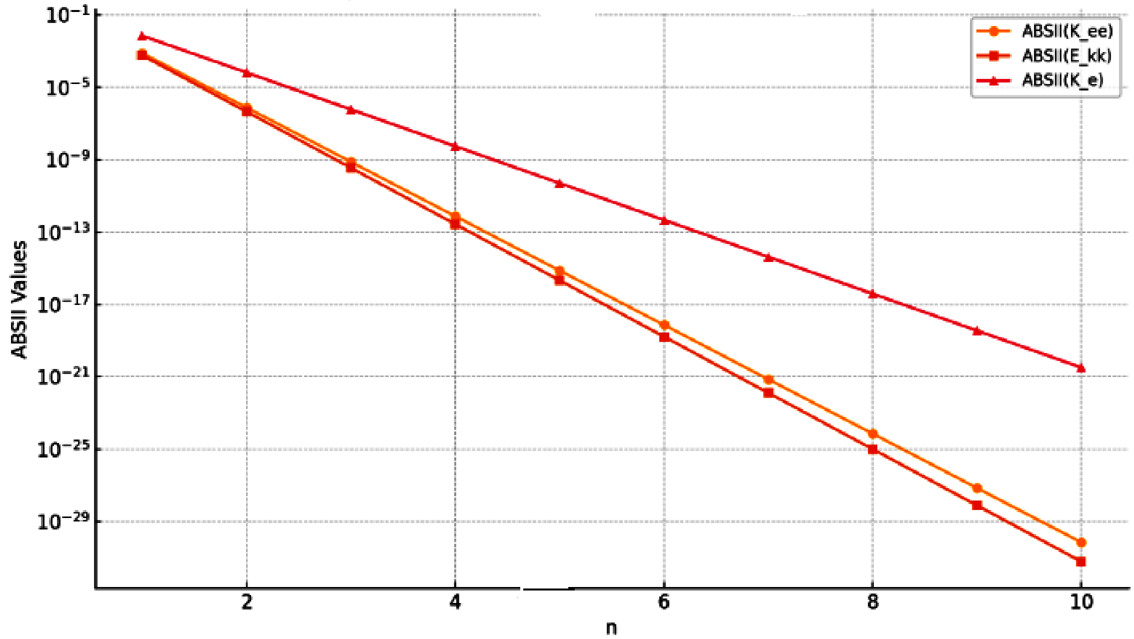

Figure 5: Comparison of atom bond sum connectivity index for PEK, PEKK and PEEK.

Results and Discussion:

The findings from our study on the Multiplicative Atom Bond Sum Connectivity Index for Poly-ether ketone, Poly-ether ketone ketone, and Poly-ether ether ketone shed light on the intricate relationship between molecular structure and performance. By diving deep into these connectivity indices, we've uncovered valuable insights that could significantly impact how these materials are understood and utilized. The ability to predict how these polymers will behave in different situations can help researchers and engineers make smarter choices when selecting materials. This means that the insights gained here could lead to more innovative designs and applications, paving the way for materials that are not only high-performing but also more sustainable. Ultimately, our work serves as a stepping stone for future explorations into optimizing polymer properties, a crucial endeavor in today's fast-paced technological landscape.

Conclusion:

To wrap up, our investigation into the Multiplicative Atom Bond Sum Connectivity Index has revealed just how crucial these connectivity measures are in understanding the behavior of Poly-ether ketone, Poly-ether ketone ketone, and Poly-ether ether ketone. These metrics offer a fresh perspective on molecular interactions, allowing us to grasp the nuances of how these materials perform. As the demand for advanced materials continues to grow, the insights from this research hold significant promise. By integrating what we've learned into the design and engineering of new materials, we can contribute to the development of cutting-edge polymers that meet the challenges of tomorrow. Together, we're not just advancing material science we're laying the groundwork for sustainable innovations that could reshape multiple industries.

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Author's Declaration:

The authors declare that there is no conflict of interest regarding the publication of this paper. All data generated or analyzed during this study are included in this published article, and no additional datasets were used.

Authors' Contribution Statement:

1. **U. Farooq**: Conceptualization, Methodology, Writing - Original Draft, Data Curation.
2. **F. Chudhary**: Supervision, Reviewing and Editing, Validation.

Both authors contributed equally to the development of this manuscript and have approved the final version for submission

Data Availablity: All data available in manuscript.

Conflicts of Intrest: On behalf of all authors, the corresponding author states that there is no conflict of interest.

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