Research Article

Exact Distance-Based Topological Indices Of Double Star Double Fanbell Graphs With Applications In Chemical Graph Theory, QSPR/QSAR Modeling, And Drug Discovery

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Abstract

The topological indices are fundamental tools in chemical graph theory with the aim of numerically describing the structural properties of molecular graphs and also predicting physicochemical and biological parameters. In this paper, we present a new graph family called Double Star Double Fanbell (BSDF) which consists of double star graph with each pendant vertex added with a double fan graph. Eight important distance based topological indices are considered, namely Wiener index, Hyper-Wiener index, Harary index, Reciprocal Complementary Wiener index, Wiener Polarity index, Terminal Wiener index, Reverse Wiener index, and Reciprocal Reverse Wiener index are considered and exact closed-form expressions are obtained. The analytical formulations are derived by a systematic distance-partitioning method and written in terms of the graph parameters, which allows the formula to be computed efficiently for any graph size without a need for any repeated shortest-path computations.

In addition to their mathematical importance, the calculated topological descriptors are useful molecular descriptors in Chemical Graph Theory, in which atoms are depicted as vertices, and chemical bonds as edges. These descriptors can be used effectively in Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) models to predict molecular stability, boiling point, melting point, solubility, lipophilicity, biological activity, toxicity and pharmacokinetic properties. Moreover, the proposed BSDF graph provides a proper model for the highly branched organic compounds, dendrimer, hyperbranched polymers, and functional nanomaterials. Expressions obtained in this work are in an exact form, which is very appealing for large scale molecular databases, virtual screening, cheminformatics and AI-assisted drug discovery. Therefore, the suggested graph is not only playing a theoretical role in advancement of graph theory but also in the present day computational chemistry and pharmaceutical research.

Keywords: Double Star Double Fanbell graph; Distance-based topological indices; Molecular descriptors; Chemical graph theory; QSPR/QSAR modeling; Wiener index; Hyper-Wiener index; Harary index; Computational drug discovery.

1. Introduction

In chemistry, biology, computer science, communication networks and material science, complex structures have become a field of study that relies heavily on graph theory for modeling and analysis. In the discipline of chemistry known as chemical graph theory, the structure of a chemical molecule is modeled as a graph with vertices corresponding to atoms, and edges representing chemical bonds. This representation helps to convert molecular structures into mathematical objects, and can be used to study the structural features using graph-theoretic descriptors, called **topological indices**. These numerical invariants are important for theoretical chemistry and cheminformatics for representing information from molecular connectivity and geometry without having to perform costly quantum chemical calculations.

In the many kinds of graph invariants suggested in the literature, the distance-based topological indices have a special place in the description of the overall structural properties of molecular graphs. Distance-based indices take into account the shortest-path distance between pairs of vertices in addition to local connectivity, which is not accounted for in degree-based indices. The

classical indices like Wiener index, Hyper-Wiener index, Harary index, Reciprocal Complementary Wiener index, Wiener Polarity index, Terminal Wiener index, Reverse Wiener index and Reciprocal Reverse Wiener index have been shown to have great predictive power for experimentally measured physicochemical and biological properties of molecules.

Such indices are not only relevant to graph theory but also to related fields like Quantitative Structure-Property Relationship (QSPR) and Quantitative Structure-Activity Relationship (QSAR) studies. QSPR and QSAR methodologies use mathematical descriptors derived from the molecular graph to build predictive models of molecular properties and biological activities. These descriptors have been used to estimate the boiling point, melting point, density, viscosity, solubility, molecular stability, lipophilicity, toxicity, pharmacokinetic behavior, and biological activity of chemical compounds with success. As a result, topological indices have emerged as an essential molecular descriptor in computational chemistry, molecular informatics and pharmaceutical sciences.

The emergence of computer-aided drug discovery (CADD) and artificial intelligence in recent years greatly accelerated the need for effective molecular descriptors that can capture the complicated molecular architecture. Modern Virtual Screening platforms analyze millions of candidate molecules before they are synthesized in the laboratory and for these systems, computationally inexpensive yet informative descriptors are needed. Numerical representations of the distance-based topological indices satisfy these requirements, as they can be directly incorporated into machine learning algorithms, QSPR/QSAR models and molecular similarity analyses. These descriptors can be very useful for lead optimization, toxicity prediction, drug repurposing, and compound identification in the field of bioactivity.

Researchers continue to develop new graph families whose structures bear strong similarity to the complex molecular structures with these developments acting as motivation. Mathematical study of the new graph structure gives exact analytical expressions for the new topological indices, which adds a new dimension to graph theory and its use in chemistry. Closed-form formulas do not require repeated shortest-path calculations, and are able to evaluate molecular descriptors for arbitrary large graphs efficiently.

This paper proposes a new graph family called the Double Star Double Fanbell (BSDF) graph, which is a combination of structural attributes of double star and double fanbell graphs, and a mathematical model. Because of its highly branched and symmetric structure, the BSDF graph is well suited to represent branched organic molecules, dendritic polymers, macromolecular compounds and functional nanoscale structures. This kind of graph models is especially appropriate to study how branchings affect the properties of a molecule and/or its biological behaviour. In this paper we will consider only finite, undirected, connected and simple graphs. Let G be a graph, (V, E), the number of vertices and number of edges of the graph will be denoted by $|V(G)|$ and $|E(G)|$ respectively. If $u, v \in V(G)$, length of the shortest distance between u and v in G is denoted by $d_G(u, v)$, we simply denote it by $d(u, v)$ if there is no ambiguity in the graph under consideration. The eccentricity of a vertex u in a graph G is $e(u) = \max\{d(u, v): v \in V(G)\}$he radius (resp. diameter) of G is $r = rad(G) = \min\{e(v): v \in V(G)\}$esp. $d = diam(G) = \max\{e(v): v \in V(G)\}$A vertex with degree 1 is called a pendent vertex or terminal node or leaf node or leaf in a graph. Definitions which are not seen here can be referred in [3] and [4].

A topological index is a numerical index that has been calculated from the structure of a graph. Indices are quantities which describe the structure of a graph. Graph techniques have many applications in various fields such as Chemistry, Physics, Biology, Computer science, etc. The Wiener index, also called the ''Wiener number'', is the distance based topological index that was introduced by Harry Wiener, a chemist in 1947 [18]. Wiener index which is widely used based on the chemical applications of graph theory which counts the number of bonds between pairs of atoms and sum the distance between all pairs by generating a distance matrix [14]. The Wiener index is defind by the sum of distances between all unordered pairs of vertices of a graph G,

$$W(G) = \sum_{u,v \in V(G)} d(u, v).$$

The hyper-Wiener index is the generalization of the Wiener index introduced by Milan Randić in 1993 [17] and is defind as follows :

$$WW(G) = \frac{1}{2} \sum_{u,v \in V(G)} [d(u, v) + d(u, v)^2].$$

In [15] Plavšić et. al., and in [10] Ivancine et. al., independently introduced the Harary index, in honor of Frank Harary. For the graph G, the Harary index is defined as the reciprocal of the Wiener index, and denoted by

$$H(G) = \sum_{u,v \in V(G)} \frac{1}{d(u, v)}.$$

In[9,11] Ivancine et. al., introduced the Reciprocal Complementary Wiener index, denoted by $RCW(G)$ and given by

$$RCW(G) = \sum_{u,v \in V(G)} \frac{1}{d + 1 - d(u, v)},$$

where d is the diameter of a graph G.

The Wiener Polarity index W_P of a graph G, is introduced by Wiener in 1947 [6], is the number of unordered pairs of vertices of G such that the distance between u and v is 3,

$$W_P(G) = |\{(u,v) \mid d(u,v) = 3, u, v \in V(G)\}|.$$

The Terminal Wiener index of a graph G is defined by Gutman et.al., in [8] , as the sum of distance between all pairs of pendent vertices of G,

$$TW(G) = \sum_{\substack{u,v \in V(G) \\ deg(u)=deg(v)=1}} d(u,v).$$

The Reverse Wiener index was proposed by Balaban et. al., in 2000 [2], is defined as follows

$$\wedge(G) = \frac{n(n-1)d}{2} - W(G),$$

where $n = |V(G)|$ and d is the diameter of G.

In [12], the Reciprocal Reverse Wiener (RRW) index $R\wedge(G)$ of a connected graph G is defined as

$$R\wedge(G) = \begin{cases} \sum_{u,v \in V(G)} \frac{1}{d - d(u,v)}, & \text{for } 0 < d(u,v) < d, \\ 0, & \text{for otherwise.} \end{cases}$$

where d is the diameter of a graph G.

In [13] double star and bistar graphs are definded. A double star is a graph obtained by joining a edge to center of $K_{1,m}$ and $K_{1,n}$ for $n > m \geq 2$ and it is denoted by $B_{m,n}$. If $m = n$ in the double star graph, it is called as bistar graph and denoted by $B_{n,n}$, see Figure 1 for $B_{4,5}$.

In [16] fan graph and double fan graph are defined. A fan graph $F_{m,n}$ is defined as the graph join $\overline{K}_m + P_n$, where $\overline{K}_m$ is the empty graph on m vertices and P_n is the path on n vertices. The case $m = 1$ corresponds to the usual fan graph $F_{1,n}$, while $m = 2$ corresponds to the double fan graph, see Figure 2 for $F_{1,4}$ and $F_{2,4}$.

Figure 1. Double Star Graph $B_{4,5}$

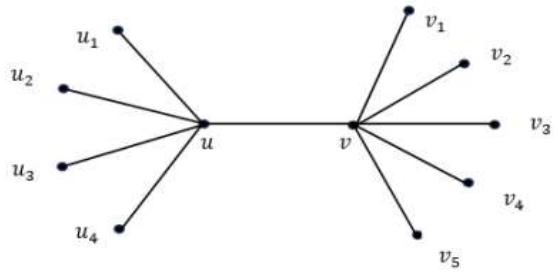
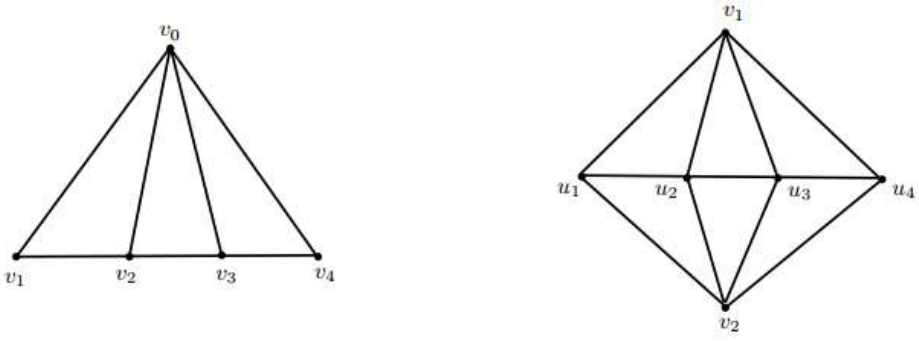


Figure 2. Fan and Double Fan Graph

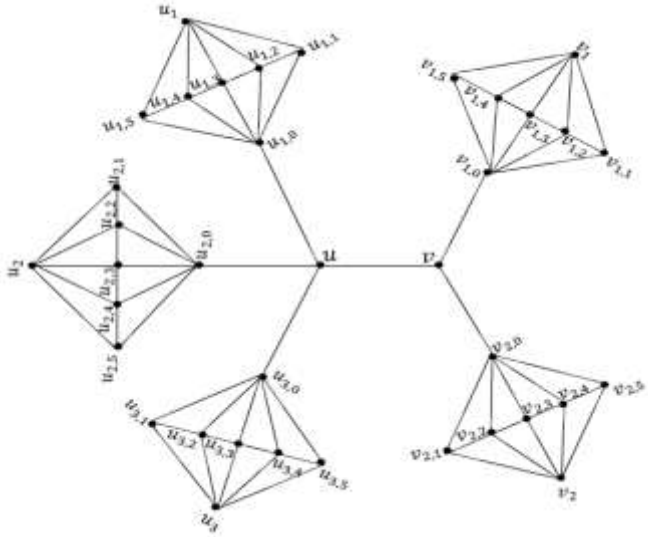


2. Indices of a Double Star Double Fanbell Graph.

In this section, we introduce double star double fanbell graph $BSDF_{r_1,r_2,\ldots,r_{m+n}}$ which is similar to double star starbell graph [1] and also we derive some results for distance-based topological indices W(G), WW(G), H(G), RCW(G), $W_P(G)$, TW(G), $\wedge(G)$ and $R\wedge(G)$, where G is a double star double fanbell graph.

Definition 2.1. The double star double fanbell graph $\mathrm{BSDF}_{\mathrm{r_1,r_2,\ldots,r_{m+n}}}$ is a graph obtained from double star graph $\mathrm{B_{m,n}}$ and $\mathrm{m+n}$ double fan graph $\mathrm{F_{2,r_i}}$ by augmenting the root vertex of each $\mathrm{F_{2,r_i}}$ to the $\mathrm{i^{th}}$ leaf of $\mathrm{B_{m,n}}$, where $\mathrm{r_i \geq 1}$, $\mathrm{1 \leq i \leq m+n}$ and $\mathrm{m, n \geq 2}$, see Figure 3 for $\mathrm{BSDF}_{\mathrm{r_1,r_2,\ldots,r_5}}$.

Figure 3. Double Star Double Fanbell Graph



Theorem 2.2. For $m, n \geq 2$ and $r \geq 1$ the double star double fanbell graph G, in which all double fan are of the same order. Then

(i) $W(G) = 1 + 2(r^2 + 4r + 4)\,[m(m-1) + n(n-1)] + (m+n)\,(r^2 + 5r + 13) + 5mn(r+2)^2.$

$(ii)\ WW(G) = \frac{1}{2}\,\{2 + (m+n)\,[2(11r+23) + (r-1)(3r-4)] + 2[m(m-1) + n(n-1)](5r^2 + 21r + 22) + 2mn(15r^2 + 62r + 64)\}.$

$(iii)\ H(G) \cong 1 + \frac{1}{12}\,(m+n)[(34r+31) + 3(r-1)(r+2)] + \frac{1}{120}\,[m(m-1) + n(n-1)](15r^2 + 64r + 70) + \frac{1}{210}\,mn(42r^2 + 175r + 184).$

$(iv)\ RCW(G) = \frac{1}{7} + \frac{1}{420}\,(m+n)[(274r+389) + 5(r-1)(7r-2)] + \frac{1}{120}[m(m-1) + n(n-1)](15r^2 + 64r + 70) + \frac{1}{30}mn(10r^2 + 45r + 56).$

Proof. Let $G = BSDF_{r_1,r_2,\ldots,r_{m+n}}$ be the double star double fanbell graph where each double fan graph has the same order with $r_i \geq 1$, $1 \leq i \leq m+n$ and $m, n \geq 2$. Let $r_i = r$, $i = 1,2,\ldots,m+n$. Let $V(G) = U_1 \cup U_2 \cup \cdots \cup U_m \cup V_1 \cup V_2 \cup \cdots \cup V_n \cup \{u, v\}$, where $U_i = \{u_{i,0}, u_{i,1}, \ldots, u_{i,r}\} \cup \{u_i\}$ and $V_j = \{v_{j,0}, v_{j,1}, \ldots, v_{j,r}\} \cup \{v_j\}$, $1 \leq i \leq m$ and $1 \leq j \leq n$. For $i, j = 1,2,\ldots,m$ and $p, q = 1,2,\ldots,n$ and $k, \ell = 1,2,\ldots,r$ and $s = 1,2,\ldots,r-1$ the distance between any two vertices in G are given by

$d(u,v) = d(u,u_{i,0}) = d(u_{i,0},u_{i,k}) = d(u_{i,k},u_i) = d(u_{i,s},u_{i,s+1}) = 1$,
$d(v,v_{p,0}) = d(v_{p,0},v_{p,k}) = d(v_{p,k},v_p) = d(v_{p,s},v_{p,s+1})$ = 1 ,
$d(u,v_{p,0}) = d(u_{i,0},v) = d(u,u_{i,k}) = d(v,v_{p,\ell}) = 2$,
$d(u_{i,0},u_i) = d(v_{p,0},v_p) = 2$,
$d(u_{i,k},u_{i,\ell}) = d(v_{p,k},v_{p,\ell}) = 2$,for $\ell \neq k, k \pm 1$,
$d(u_{i,0},u_{j,0}) = d(v_{p,0},v_{q,0}) = 2,$ for $i \neq j$ and $p \neq q$,

$d(u,u_i) = d(v,v_p) = 3$,
$d(u_{i,0},u_{j,k}) = d(v_{p,0},v_{q,k}) = 3$, for $i \neq j$ and $p \neq q$,
$d(u,v_{p,k}) = d(u_{i,k},v) = d(u_{i,0},v_{p,0}) = 3$,
$d(u,v_p) = d(u_i,v) = d(u_{i,0},v_{p,k}) = d(u_{j,k},v_{q,0}) = 4$,
$d(u_{i,k},u_{j,\ell}) = d(v_{p,k},v_{q,\ell}) = 4$, for $i \neq j$ and $p \neq q$,
$d(u_i,u_{j,0}) = d(v_p,v_{q,0}) = 4$, for $i \neq j$ and $p \neq q$,
$d(u_i,u_{j,k}) = d(v_p,v_{q,\ell}) = 5$, for $i \neq j$ and $p \neq q$,
$d(u_i,v_{p,0}) = d(u_{i,0},v_p) = d(u_{i,k},v_{p,\ell}) = 5$,
$d(u_i,u_j) = d(v_p,v_q) = d(u_{i,k},v_p) = d(u_i,v_{p,\ell}) = 6$,
$d(u_i,v_p) = 7$.

Here $diam(G) = 7$ and the distance between any pair of vertices varies from $1,2,\ldots,diam(G)$. The number of pair of vertices receives distance $1, 2, 3, 4, 5, 6$ and 7 are $1 + m + n + 2mr + 2nr + m(r-1) + n(r-1)$, $2m + 2n + mr + nr + \binom{m}{2} + \binom{n}{2} + m\binom{r-1}{2} + n\binom{r-1}{2}$, $m + n + mr + nr + 2\binom{m}{2}r + 2\binom{n}{2}r + mn$, $m + n + 2mnr + r^2\binom{m}{2} + r^2\binom{n}{2} + 2\binom{m}{2} + 2\binom{n}{2}$, $mnr^2 + 2mn + 2r\binom{m}{2} + 2r\binom{n}{2}$, $2mnr + \binom{m}{2} + \binom{n}{2}$ and mn respectively. By using these we derive the following

$$
\begin{aligned}
W(G) &= 1 + m + n + 2mr + 2nr + m(r-1) + n(r-1) \\
&\quad + [2m + 2n + mr + nr + \binom{m}{2} + \binom{n}{2} + m\binom{r-1}{2} + n\binom{r-1}{2}]2 \\
&\quad + [m + n + mr + nr + 2\binom{m}{2}r + 2\binom{n}{2}r + mn]3 + [m + n + 2mnr \\
&\quad + r^2\binom{m}{2} + r^2\binom{n}{2} + 2\binom{m}{2} + 2\binom{n}{2}]4 + [mnr^2 + 2mn + 2r\binom{m}{2} \\
&\quad + 2r\binom{n}{2}]5 + [2mnr + \binom{m}{2} + \binom{n}{2}]6 + 7mn \\
&= 1 + 2(r^2 + 4r + 4)[m(m-1) + n(n-1)] + (m+n)(r^2 + 5r + 13) \\
&\quad + 5mn(r+2)^2.
\end{aligned}
$$

$$
\begin{aligned}
WW(G) &= \frac{1}{2}\{[1 + m + n + 2mr + 2nr + m(r-1) + n(r-1)](1 + 1^2) \\
&\quad + [2m + 2n + mr + nr + \binom{m}{2} + \binom{n}{2} + m\binom{r-1}{2} \\
&\quad + n\binom{r-1}{2}](2 + 2^2) + [m + n + mr + nr + 2\binom{m}{2}r + 2\binom{n}{2}r \\
&\quad + mn](3 + 3^2) + [m + n + 2mnr + r^2\binom{m}{2} + r^2\binom{n}{2} + 2\binom{m}{2} \\
&\quad + 2\binom{n}{2}](4 + 4^2) + [mnr^2 + 2mn + 2r\binom{m}{2} + 2r\binom{n}{2}](5 + 5^2) \\
&\quad + [2mnr + \binom{m}{2} + \binom{n}{2}](6 + 6^2) + [mn](7 + 7^2)\} \\
&= \frac{1}{2}\{2 + (m+n)[2(11r + 23) + (r-1)(3r-4)] + 2[m(m-1) \\
&\quad + n(n-1)](5r^2 + 21r + 22) + 2mn(15r^2 + 62r + 64)\}.
\end{aligned}
$$

$$H(G) = 1 + m + n + 2mr + 2nr + m(r-1) + n(r-1) + [2m + 2n + mr + nr + \binom{m}{2} + \binom{n}{2} + m\binom{r-1}{2} + n\binom{r-1}{2}]\frac{1}{2} + [m + n + mr + nr + 2\binom{m}{2}r + 2\binom{n}{2}r + mn]\frac{1}{3} + [m + n + 2mnr + r^2\binom{m}{2} + r^2\binom{n}{2} + 2\binom{m}{2} + 2\binom{n}{2}]\frac{1}{4} + [mnr^2 + 2mn + 2r\binom{m}{2} + 2r\binom{n}{2}]\frac{1}{5} + [2mnr + \binom{m}{2} + \binom{n}{2}]\frac{1}{6} + \frac{1}{7}mn = 1 + \frac{1}{12}(m+n)[(34r + 31) + 3(r-1)(r+2)] + \frac{1}{120}[m(m-1) + n(n-1)](15r^2 + 64r + 70) + \frac{1}{210}mn(42r^2 + 175r + 184).$$

$$RCW(G) = [1 + m + n + 2mr + 2nr + m(r-1) + n(r-1)]\frac{1}{7} + [2m + 2n + mr + nr + \binom{m}{2} + \binom{n}{2} + m\binom{r-1}{2} + n\binom{r-1}{2}]\frac{1}{6} + \left[m + n + mr + nr + 2\binom{m}{2}r + 2\binom{n}{2}r + mn\right]\frac{1}{5} + \left[m + n + 2mnr + r^2\binom{m}{2} + r^2\binom{n}{2} + 2\binom{m}{2} + 2\binom{n}{2}\right]\frac{1}{4} + \left[mnr^2 + 2mn + 2r\binom{m}{2} + 2r\binom{n}{2}\right]\frac{1}{3} + \left[2mnr + \binom{m}{2} + \binom{n}{2}\right]\frac{1}{2} + mn = \frac{1}{7} + \frac{1}{420}(m+n)[(274r + 389) + 5(r-1)(7r-2)] + \frac{1}{120}[m(m-1) + n(n-1)](15r^2 + 64r + 70) + \frac{1}{30}mn(10r^2 + 45r + 56).$$ □

Corollary 2.3. For the double star double fanbell graph G with $m, n \geq 2$ and $r \geq 1$, $W_P(G) = (m+n)(1+r) + [m(m-1) + n(n-1)]r + mn$.

Proof. The number of 3 distance pair of vertices is $m + n + mr + nr + 2\binom{m}{2}r + 2\binom{n}{2}r + mn$ by Theorem 2.2. So, $W_P(G) = (m+n)(1+r) + [m(m-1) + n(n-1)]r + mn$.

□

Corollary 2.4. For $m, n \geq 2$ and $r = 1$ the double star double fanbell graph G has the terminal Wiener index as $TW(G) = 3[m(m-1) + n(n-1)] + 7mn$.

Proof. For $m, n \geq 2$ and $r = 1$, by Theorem 2.2 we have $TW(G) = \left[\binom{m}{2} + \binom{n}{2}\right]6 + [mn]7 = 3[m(m-1) + n(n-1)] + 7mn$.

Lemma 2.5. For the double star double fanbell graph G with $m, n \geq 2$ and $r \geq 1$, $\wedge(G) = \frac{7}{2}[(m+n)(r+2) + 2][(m+n)(r+2) + 1] - [1 + 2(r^2 + 4r + 4)[m(m-1) + n(n-1)] + (m+n)(r^2 + 5r + 13) + 5mn(r+2)^2]$.

Proof. For $m, n \geq 2$ and $r \geq 1$, $|V(G)| = (m+n)(r+2) + 2$, the diameter of G is 7 (that is, $d = 7$) by Theorem 2.2 and $W(G) = 1 + 2(r^2 + 4r + 4)[m(m-1) + n(n-1)] + (m+n)(r^2 + 5r + 13) + 5mn(r+2)^2$, hence $\wedge(G) = \frac{7}{2}[(m+n)(r+2) + 2][(m+n)(r+2) + 1] - [1 + 2(r^2 + 4r + 4)[m(m-1) + n(n-1)] + (m+n)(r^2 + 5r + 13) + 5mn(r+2)^2]$. □

Lemma 2.6. For the double star double fanbell graph G with $m, n \geq 2$ and $r \geq 1$,

$$R\wedge(G) = \frac{1}{6} + \frac{1}{60}(m+n)[(47r + 69) + 2(r-1)(3r-1)] + \frac{1}{60}[m(m-1) + n(n-1)](10r^2 + 45r + 56) + \frac{1}{12}mn(6r^2 + 32r + 15).$$

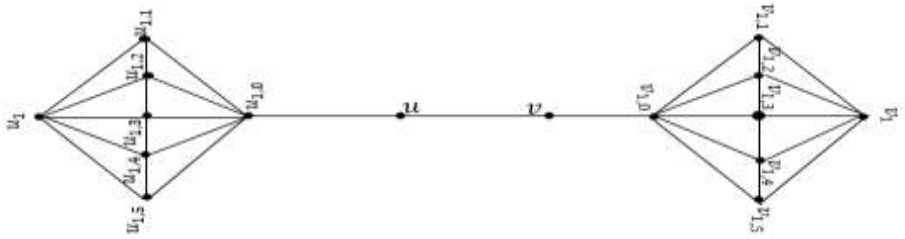
Proof. For $m, n \geq 2$ and $r \geq 1$, the double star double fanbell graph G has the diameter $d = 7$ and the distance between any pair of vertices varies from $0 < d(u,v) < d$. The number of pair of vertices receives distance 1, 2, 3, 4, 5 and 6 are $1 + m + n + 2mr + 2nr + m(r-1) + n(r-1)$, $2m + 2n + mr + nr + \binom{m}{2} + \binom{n}{2} + m\binom{r-1}{2} + n\binom{r-1}{2}$, $m + n + mr + nr + 2\binom{m}{2}r + 2\binom{n}{2}r + mn$, $m + n + 2mnr + r^2\binom{m}{2} + r^2\binom{n}{2} + 2\binom{m}{2} + 2\binom{n}{2}$, $mnr^2 + 2mn + 2r\binom{m}{2} + 2r\binom{n}{2}$ and $2mnr + \binom{m}{2} + \binom{n}{2}$ respectively.

Then we have

$$
\begin{aligned}
R \wedge (G) = {} & [1 + m + n + 2mr + 2nr + m(r-1) + n(r-1)]\frac{1}{6} + [2m \\
& + 2n + mr + nr + \binom{m}{2} + \binom{n}{2} + m\binom{r-1}{2} + n\binom{r-1}{2}]\frac{1}{5} \\
& + [m + n + mr + nr + 2\binom{m}{2}r + 2\binom{n}{2}r + mn]\frac{1}{4} + [m + n \\
& + 2mnr + r^2\binom{m}{2} + r^2\binom{n}{2} + 2\binom{m}{2} + 2\binom{n}{2}]\frac{1}{3} + [mnr^2 \\
& + 2mn + 2r\binom{m}{2} + 2r\binom{n}{2}]\frac{1}{2} + 2mnr + \binom{m}{2} + \binom{n}{2} \\
= {} & \frac{1}{6} + \frac{1}{60}(m+n)[(47r + 69) + 2(r-1)(3r-1)] \\
& + \frac{1}{60}[m(m-1) + n(n-1)](10r^2 + 45r + 56) \\
& + \frac{1}{12}mn(6r^2 + 32r + 15).
\end{aligned}
$$

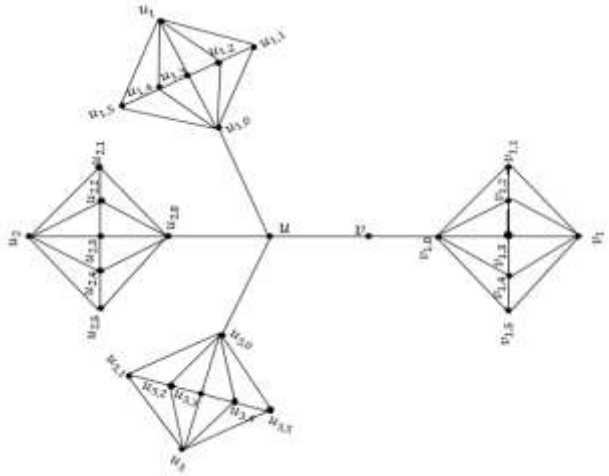
Remark 2.1. In Theorem 2.2, when $m = n = 1$ and $r \geq 1$, we get a particular graph G as shown in the Figure 4, the proof of Theorem 2. 2 is still valid for G.

Figure 4. Double Star Double Fanbell Graph G



Remark 2.2. In Theorem 2.2, either any one of m, n is 1 and $r \geq 1$, without loss of generality $m = 1$ and $n \geq 2$, we get a particular graph G' as shown in the Figure 5, the proof of Theorem 2.2 is still valid for G'.

Figure 5. Double Star Double Fanbell Graph G'



Note 2.1. For fixed r, the graph G and G', mentioned in Remark 2.1 and Remark 2.2, respectively, we have

$$
\begin{aligned}
W_P(G) &= W_P(G') = W_P\left(BSDF_{r_1,r_2,\ldots,r_{m+n}}\right) \\
TW(G) &= TW(G') = TW\left(BSDF_{r_1,r_2,\ldots,r_{m+n}}\right) \\
\wedge(G) &= \wedge(G') = \wedge\left(BSDF_{r_1,r_2,\ldots,r_{m+n}}\right)
\end{aligned}
$$

$$R \wedge (G) = R \wedge (G') = R \wedge \left(BSDF_{r_1, r_2, \ldots, r_{m+n}}\right)$$

3. Applications

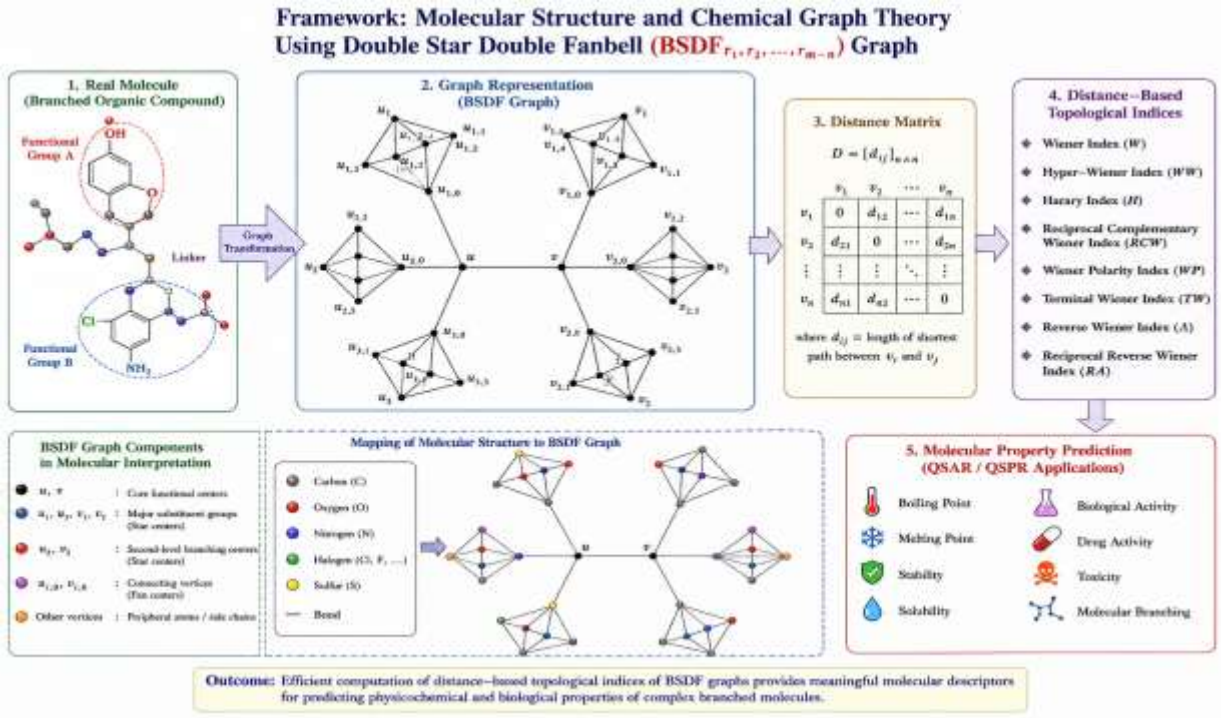
The proposed Double Star Double Fanbell (BSDF) graph is an effective mathematical model for molecular architectures that are very branched in structure, which are found in chemical graph theory. The BSDF graph can be used to interpret it as a molecular structure with vertices as atoms and the edges as chemical bonds as shown in the image below. Due to its highly symmetric and branched structure, it is capable of being modeled as a dendritic molecule, hyperbranched polymers, functional nanomaterials and more complex organic molecules. Closed-form expressions for the Wiener, Hyper-Wiener, Harary, Reciprocal Complementary Wiener, Wiener Polarity, Terminal Wiener, Reverse Wiener and Reciprocal Reverse Wiener indices were obtained, which are useful for computing molecular descriptors in an efficient manner, without the need to repeat the shortest-path calculation.

The calculated topological indices can be directly used as structural descriptors in Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) studies. These descriptors help to predict certain key physicochemical and biological properties such as molecular stability, boiling point, melting point, solubility, lipophilicity, toxicity, pharmacokinetic activity and biological activity. Therefore, the proposed BSDF graph is a valuable mathematical tool for virtual screening, molecular similarity analysis, lead optimization and computer-aided drug discovery.

Additionally, the analytical formulas derived in this work are precisely reduced in computational complexity of large molecular datasets. The descriptors can be computed directly from the parameters derived from the graph and are thus well suited for cheminformatics databases, molecular prediction systems based on artificial intelligence and for high throughput computational chemistry applications. Thus, the BSDF graph makes a useful link between graph theory and the current application of modern pharmaceutical research by generating reliable and computational efficient molecular descriptors. In Figure 6, this is shown in a conceptual way with the Double Star Double Fanbell graph. This representation has each vertex as an atom, and each edge as a chemical bond, so that the graph can represent the connectivity pattern of a branched molecular structure. The backbone portion is shown as a double-star framework while the side chains or functional groups are modeled as double fanbell arms attached to the double-star. These representations are especially useful for molecules that have more than one branching point and are symmetrical.

The structural features depicted in Figure 6 allow the calculated distance-based topological indices to be used to measure the branching, connectivity and general complexity of molecules. These numerical descriptors can then be used to build a QSPR/QSAR model for the estimation of molecular properties or biological activities. Therefore, the practical applicability of the proposed BSDF graph as a mathematical model for molecular design, computational chemistry, cheminformatics, and AI-assisted drug discovery is highlighted in Figure 6.

Figure 6. Molecular Structure Using Double Star Double Fanbell Graph



4. Conclusion

A new family of graphs, Double Star Double Fanbell (BSDF), is presented in this paper, which is a structural fusion of Double Star and Double Fan graphs. Eight important distance based topological indices have been obtained as closed-form expressions, namely the Wiener index, Hyper-Wiener index, Harary index, Reciprocal Complementary Wiener index, Wiener Polarity index, Terminal Wiener index, Reverse Wiener index and Reciprocal Reverse Wiener index. Derivations were achieved systematically via distance-partitioning, leading to analytical formulas which can evaluate shortest-paths efficiently for any graph, without repeated computation.

The expressions so obtained are used to help the theory building of chemical graph theory and are exact mathematical descriptors of a new class of graphs, the graph family. These descriptors describe molecular connectivity and branching, and are well suited to be used in QSPR/QSAR modelling, prediction of molecular properties, cheminformatics, virtual screening, and computer-aided drug discovery. The proposed BSDF graph also gives a good mathematical representation of highly branched organic compounds, dendrimers, hyperbranched polymers and functional nanomaterials. Future research could include developing other degree-based, eccentricity-based, entropy-based, and spectral topological indices for the BSDF graph, adding weight and/or direction to the graph structure of the BSDF and exploring its application in pharmaceutical research and drug discovery. This suggested graph family hence offers a sincere groundwork for future theoretical studies and applications in graph theory, computational chemistry and drug discovery.

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