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Intelligent Computing of Mathematical Properties of a Bio-Nanorobotic Systems Component, C_{70} Nanoparticle

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Abstract. This paper introduces a new methodology to compute a set of optimal mathematical properties of C_{70} fullerene nanoparticle, which has some potential applications in bio-nanorobotic systems, using graph algorithms according to the following process: (1) demonstrating graph-based structure of the nanoparticle based on its real structural data, and (2) computing the mathematical Wiener and hyper-Wiener indices as well as their respective Hosoya and hyper-Hosoya polynomials based on dynamic programming. The computed results revealed a good agreement with mathematical equations between indices and polynomials.

Keywords: C_{70} nanoparticle, Graph algorithms, Dynamic programming, Bio-nanorobotic systems.

1. Introduction

Recent advances in understanding fullerenes properties have raised the possibility of their applications in relation with bio-nanorobotic systems [1, 2]. Reaching to the many of these applications depends on understanding of their structural properties. Computational studies can make clear understanding of structural properties of complex nanoparticles in order to facilitate bottom-up construction of potential bio-nanorobotic systems. In this paper, we have focused on fullerene C_{70} as one of the sophisticated nanoparticles with versatile properties. Fullerene C_{70} is a nanoparticle which is composed of 70 equivalent carbon atoms arranged as a hollow cage in the form of a rugby-ball, egg-shaped structure with 12 pentagons and 25 hexagons joined together [3]. The rugby-ball shaped structure of C_{70} was first proposed in 1985 by Heath *et al*. [4] and then confirmed by experiment [5]. This nanoparticle also exists in the natural environments, such as in soot [6] and astronomical environments (meteorites) [7]. In this paper, the mathematical indices of C_{70} including Wiener and hyper-Wiener as well as Hosoya and Hyper-Hosoya polynomials have been computed with dynamic programming [8] of graph algorithms. These optimal mathematical indices are in relation with applications of C_{70} nanoparticle. As organization of this paper, we have presented: (1) a graph-based model of C_{70}'s structure using its real experimental data in section 2, (2) the mathematical formulas of the optimal indices and polynomials of C_{70} in section 3, and (3) computational calculations of the mathematical indices and polynomials of C_{70} in section 4. Computational bio-nanotechnology can solve many problems beyond the complex structures and mechanisms in the nanoworld and uncover the possibility that they could find applications in potentially human made bio-nanosystems.

2. Mathematical model of C_{70}'s structure

The atomic sites of C_{70} nanoparticle have been classified into 5 different atomic sites with three clear groups of bonds among them as: (1) single bonds (i.e. a-a, b-c, c-d and e-e bonds), (2) intermediate bonds (i.e. d-d and d-e bonds) and (3) double bonds (i.e. a-b and c-c bonds) with about 1.46 Å, 1.42 Å and 1.40 Å

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lengths for each group respectively [9]. According to this classification of C_{70}'s bonds, a simplified and mathematical graph-based model of C_{70} nanoparticle can be depicted as Fig. 1. In Fig.1, the single, intermediate and double bonds are in purple, green, and orange colours respectively. As it can be seen from Fig. 1, there are 105 bonds in structure of C_{70} nanoparticle including 55 single, 30 intermediate and 20 double bonds [10]. C_{70} has a stable structure which is as its hexagon-pentagon structure satisfies the Isolated Pentagon Rule (IPR) [11]. The IPR states that the most stable fullerenes will be those in which all the pentagons are surrounded entirely by hexagons [11].

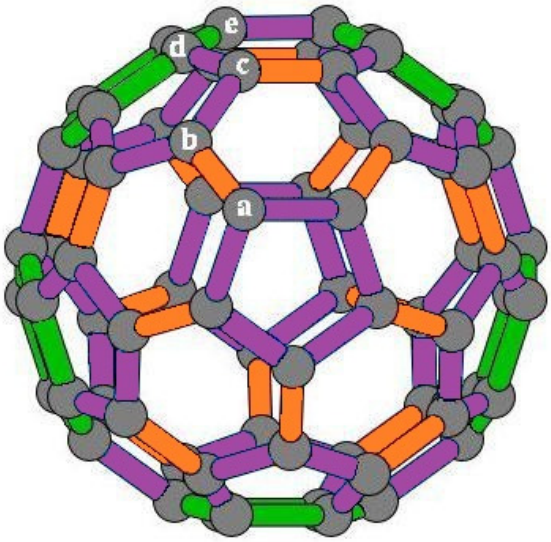

Fig. 1: The mathematical graph-based model of C_{70} nanoparticle with three kinds of bonds.

3. Mathematical formulas of C_{70}'s indices and polynomials

Let G be a connected and undirected graph with vertex set V (G) and edge set E (G). We use |V (G)| and |E (G)| to denote the cardinality of V and E respectively. Over a half century ago, the oldest topological index of G was introduced by Harold Wiener as the Wiener index [12]. The Wiener index of G, W (G), is known the sum of distances between all pairs of vertices in G and defined by:

$$W(G) = \sum_{\substack{\{u, v\} \subseteq V(G), \\ u<v}} d(u, v). \tag{1}$$

The amount of d (u, v) denotes the length of minimal path connecting u and v [13]. The Wiener index is correlated with numerous physico-chemical properties of organic compounds which are important in their applications, such as boiling point, heat of evaporation, heat of formation, chromatographic retention times, surface tension, vapor pressure, partition coefficients, etc [1]. Another modification of the Wiener index was defined as the hyper-Wiener index of G [14]:

$$WW(G) = (1/2) \sum_{\substack{\{u, v\} \subseteq V(G), \\ u<v}} \left(d(u, v)^2 + d(u, v)\right). \tag{2}$$

The x-analogue of the Wiener index is the Hosoya polynomial. It was first introduced by Hosoya [15] for a graph of G as:

$$H(G) = H(G, x) = \sum_{k \neq 0} d(G, k)\, x^k. \tag{3}$$

The amount of d (G, k) is the number of pairs of vertices in the graph G that are k distance apart. Perhaps the most interesting property of H (G, x) is its relationships with Wiener index [16] and hyper-Wiener index [17] that are defined as:

$$W(G) = H'(G, 1) \tag{4}$$

$$WW(G) = H'(G, 1) + (1/2)\, H''(G, 1). \tag{5}$$

The H' (G, 1) and H'' (G, 1) are the first and second derivatives of H (G, x) evaluated at x = 1 respectively. From Equation (5), hyper-Hosoya polynomial is integrated as [18]:

$$HH(G) = HH(G, x) = \int \left(H'(G, x) + (1/2) \times H''(G, x)\right) dx. \quad (6)$$

The hyper-Hosoya polynomial is in relationship with hyper-Wiener index as [18]:

$$WW(G) = HH'(G, 1), \quad (7)$$

where HH' (G, 1) is the first derivative of HH (G, x) evaluated at x = 1.

4. Computational Calculations of C_{70}'s Mathematical Indices and Polynomials

In this section we have computed the mathematical indices and polynomials of C_{70} nanoparticle, mentioned in previous section, using dynamic programming of graph algorithms which employ three adjacency, distance and shortest distance matrixes (Table 1).

Table 1. Definition of adjacency, distance and shortest distance matrixes of a graph G whit supposing |V (G)| = N.

Matrix	Definition
Adjacency $A[a_{ij}]_{N\times N}$	If (an edge joins vertices i and j) then $a_{ij} = 1$, zero otherwise. Obviously, if (i = = j) then $a_{ij} = 0$.
Distance $D[d_{ij}]_{N\times N}$	If (a_{ij} = =1) then d_{ij} = length of the edge between vertices i and j, otherwise $d_{ij} = \infty$. Obviously, if (i = = j) then $d_{ij} = 0$.
Shortest distance $S[s_{ij}]_{N\times N}$	s_{ij} = length of the shortest path between vertices i and j for which all intermediate vertices are in the set V. Obviously, if (i = = j) then $s_{ij} = 0$.
Each of the a_{ij}, d_{ij}, s_{ij} values is related to the value on line i and column j of their respective matrixes, $1 \le i, j \le N$.	

According to Equation (1), the Wiener index of C_{70} nanoparticle, W (C_{70}), was calculated with the following algorithm:

Input: S $[s_{ij}]_{70\times 70}$.

Output: W (C_{70}).

```
begin
    W (C70) = 0.0;
    for (i = 1 to 70)
      for (j = i to 70)
        W (C70) = W (C70) + sij;
end.
```

The matrix of S $[s_{ij}]_{70\times 70}$ is computed already using a dynamic programming algorithm called Floyd-Warshall algorithm [19] to compute shortest paths between all pairs of vertices in the graph as:

Input: D $[d_{ij}]_{70\times 70}$.

Output: S $[s_{ij}]_{70\times 70}$.

```
begin
   for (k = 1 to 70)
    for (i = 1 to 70)
      for (j = 1 to 70)
        sij = min (dij, dik+ dkj);
end.
```

The computed Wiener index of C_{70} is W (C_{70}) = 17749.9. For computing the hyper-Wiener of C_{70}, WW (C_{70}), the following algorithm was used according to the Equation (2) as:

Input: S $[s_{ij}]_{70\times 70}$.

Output: WW (C_{70}).

```
begin
```

WW (C_{70}) = 0.0;
for (i = 1 **to** 70)
for (j = i **to** 70)
WW (C_{70}) = WW (C_{70}) + (s_{ij}^2 + s_{ij});
WW (C_{70}) = (1/2) × WW (C_{70});
end.

The resulted hyper-Wiener of C_{70} is WW (C_{70}) = 85448.4. The next properties of C_{70} are the Hosoya and hyper-Hosoya polynomials of C_{70}. The following algorithm is for computing the Hosoya polynomial of C_{70}, H (C_{70}), according to Equation (3) as:

Input: S $[s_{ij}]_{70\times70}$.

Output: H (C_{70}).

begin
H (C_{70}) = 0;
for (i = 1 **to** 70)
for (j = i + 1 **to** 70)
H (C_{70}) = H (C_{70}) + ($x^{S_{ij}}$);
end.

The result is H(C_{70}) = 20 $x^{1.40}$ + 30 $x^{1.42}$ + 55 $x^{1.46}$ + 30 $x^{2.84}$ + 80 $x^{2.86}$ + 60 $x^{2.88}$ + 40 $x^{2.92}$ + 45 $x^{4.26}$ + 40 $x^{4.28}$ + 80 $x^{4.30}$ + 100 $x^{4.32}$ + 20 $x^{4.34}$ + 40 $x^{5.70}$ + 150 $x^{5.72}$ + 60 $x^{5.74}$ + 50 $x^{5.76}$ + 60 $x^{5.78}$ + 40 $x^{7.12}$ + 60 $x^{7.14}$ + 90 $x^{7.16}$ + 105 $x^{7.18}$ + 40 $x^{7.20}$ + 20 $x^{7.22}$ + 20 $x^{7.24}$ + 40 $x^{8.56}$ + 100 $x^{8.58}$ + 80 $x^{8.60}$ + 100 $x^{8.62}$ + 40 $x^{8.64}$ + 20 $x^{8.66}$ + 5 $x^{8.68}$ + 15 $x^{9.98}$ + 20 $x^{10.00}$ + 90 $x^{10.02}$ + 60 $x^{10.04}$ + 50 $x^{10.06}$ + 80 $x^{10.08}$ + 20 $x^{10.10}$ + 50 $x^{11.44}$ + 40 $x^{11.46}$ + 95 $x^{11.48}$ + 20 $x^{11.50}$ + 20 $x^{11.54}$ + 20 $x^{12.86}$ + 10 $x^{12.88}$ + 55 $x^{12.90}$ + 20 $x^{12.92}$ + 20 $x^{12.94}$ + 10 $x^{14.34}$. Meanwhile, hyper-Hosoya polynomial of C_{70}, HH (C_{70}), is computed using the following algorithm according to Equation (6) as:

Input: H (C_{70}).

Output: HH (C_{70}).

begin
H' (C_{70}) = 0; H" (C_{70}) = 0; Ž (C_{70}) = 0; HH (C_{70}) = 0;
for (each of (d (G, k) x^k) in H (C_{70}))
{ H' (C_{70}) = H' (C_{70}) + (k × d (G, k) x^{k-1});
H" (C_{70}) = H" (C_{70}) + (k × (k – 1) d (G, k) x^{k-2});}
Ž (C_{70}) = H' (C_{70}) + (1/2) × x × H" (C_{70});
for (each of (d (G, k) x^k) in Ž (C_{70}))
HH (C_{70}) = HH (C_{70}) + (d (G, k) / (k + 1)) (x^{k+1});
end.

The result is HH (C_{70}) = 24 $x^{1.40}$ + 36.3 $x^{1.42}$ + 67.65 $x^{1.46}$ + 57.6 $x^{2.84}$ + 154.4 $x^{2.86}$ + 116.4 $x^{2.88}$ + 78.4 $x^{2.92}$ + 118.35 $x^{4.26}$ + 105.6 $x^{4.28}$ + 212 $x^{4.30}$ + 266 $x^{4.32}$ + 53.4 $x^{4.34}$ + 134 $x^{5.70}$ + 504 $x^{5.72}$ + 202.2 $x^{5.74}$ + 169 $x^{5.76}$ + 203.4 $x^{5.78}$ + 162.4 $x^{7.12}$ + 244.2 $x^{7.14}$ + 367.2 $x^{7.16}$ + 429.45 $x^{7.18}$ + 164 $x^{7.20}$ + 82.2 $x^{7.22}$ + 82.4 $x^{7.24}$ + 191.2 $x^{8.56}$ + 479 $x^{8.58}$ + 384 $x^{8.60}$ + 481 $x^{8.62}$ + 192.8 $x^{8.64}$ + 96.6 $x^{8.66}$ + 24.2 $x^{8.68}$ + 82.35 $x^{9.98}$ + 110 $x^{10.00}$ + 495.9 $x^{10.02}$ + 331.2 $x^{10.04}$ + 276.5 $x^{10.06}$ + 443.2 $x^{10.08}$ + 111 $x^{10.10}$ + 311 $x^{11.44}$ + 249.2 $x^{11.46}$ + 592.8 $x^{11.48}$ + 125 $x^{11.50}$ + 125.4 $x^{11.54}$ + 138.6 $x^{12.86}$ + 69.4 $x^{12.88}$ + 382.25 $x^{12.90}$ + 139.2 $x^{12.92}$ + 139.4 $x^{12.94}$ + 76.7 $x^{14.34}$. We tested our computational results with Equations (4, 5, 7) and found a good agreement in our calculations as:

$$W(C_{70}) = H'(C_{70}, 1) = 17749.9,$$
$$WW(C_{70}) = H'(C_{70}, 1) + (1/2)\, H''(C_{70}, 1) = 85448.4,$$
$$WW(C_{70}) = HH'(C_{70}, 1) = 85448.4.$$

5. Conclusions

Computational intelligence can solve many problems beyond the complex structures and mechanisms in the nanoworld and uncover the possibility that they could find applications in potential bio-nanorobotic and nanorobotic systems. C_{70} is one of the nanoparticles with complex structure that planned in some potential nanorobotic applications. In this work, we have presented a set of computational calculations of C_{70}'s mathematical indices including Wiener and hyper-Wiener, with results of 17749.9 and 85448.4 respectively, as well as Hosoya and hyper-Hosoya polynomials of C_{70} nanoparticle. We have demonstrated that our computational results are in agreement with the mathematical relationships which are between these indices and polynomials. Some potential applications of C_{70} will need more time to become reality. Computational calculations of C_{70} might lead to solutions to problems beyond those that are only imagined today.

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7. References

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