Hindawi Publishing Corporation
Journal of Chemistry
Volume 2016, Article ID 2053293, 5 pages
http://dx.doi.org/10.1155/2016/2053293

Research Article

Hosoya Index of *L*-Type Polyphenyl Spiders

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Received 3 August 2016; Accepted 8 November 2016

Academic Editor: Somdet Srichairatanakool

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The polyphenyl system is composed of n hexagons obtained from two adjacent hexagons that are sticked by a path with two vertices. The Hosoya index of a graph G is defined as the total number of the independent edge sets of G. In this paper, we give a computing formula of Hosoya index of a type of polyphenyl system. Furthermore, we characterize the extremal Hosoya index of the type of polyphenyl system.

1. Introduction

The polyphenyl system is composed of n hexagons obtained from two adjacent hexagons that are sticked by a path P_2. Polyphenyl systems are of great importance for theoretical chemistry because they are natural molecular graph representations of benzenoid hydrocarbons [1]. Polyphenyl systems are graph representations of an important subclass of benzenoid molecules.

A topological index is a numerical quantity derived in a unambiguous manner from the structure graph of a molecule. As a graph structural invariant, it does not depend on the label or the pictorial representation of that graph. Various topological indices usually reflect the molecular size and shape. One topological index is Hosoya index, which was first introduced by Hosoya [2]. It plays an important role in the so-called inverse structure-property relationship problems. For details of Hosoya index and its applications, the readers are suggested to refer to [1, 3–5] and references therein. For other topological indices, please see [6–23], among others.

In this paper, our aim is to find the computation formula of Hosoya index of a polyphenyl system. We present some definitions and notations as follows.

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. Let e and u be an edge and a vertex of G, respectively. We will denote by $G - e$ or $G - u$ the graph obtained from G by removing e or u, respectively. Denote by N_u the set $\{v \in V(G) : uv \in E(G)\} \cup \{u\}$. Let H be a subset of $V(G)$. The subgraph of G induced by H is denoted by $G[H]$, and $G[V \setminus H]$ is denoted by $G - H$.

Two edges of G are said to be independent if they are not adjacent in G. A k-matching of G is a set of k mutually independent edges. Denote by $m(G, k)$ the number of the k-matchings of G. For convenience, let $m(G, 0) = 1$ for any graph G. The *Hosoya index* of G, denoted by $Z(G)$, is defined as

$$Z(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} m(G, k), \quad (1)$$

where n stands for the order, the number of vertices, of G and $\lfloor n/2 \rfloor$ is the integer part of $n/2$.

We denote by $d_H(G)$ hexagonal degree of a polyphenyl system graph, which is the number of hexagons sticked by three P_2's. A polyphenyl system graph G is called the polyphenyl spider (see Figure 1) if $d_H(G) = 1$ and called polyphenyl chain if $d_H(G) = 0$. Let polyphenyl chain $s(n)$ be composed of n hexagons $B_1, B_2, \ldots, B_n$ obtained from two vertices of adjacent hexagons B_i and B_{i+1} that are vertex-sticked by two end vertices of path P_2, respectively. If the two vertex sets of B_i $(i = 2, 3, \ldots, n-1)$ in $s(n)$ divided by two path P_2's both have two vertices, then it is called a linear polyphenyl chain, denoted by $l(n)$. Let $g(n), h(n)$, and $q(n)$ be induced

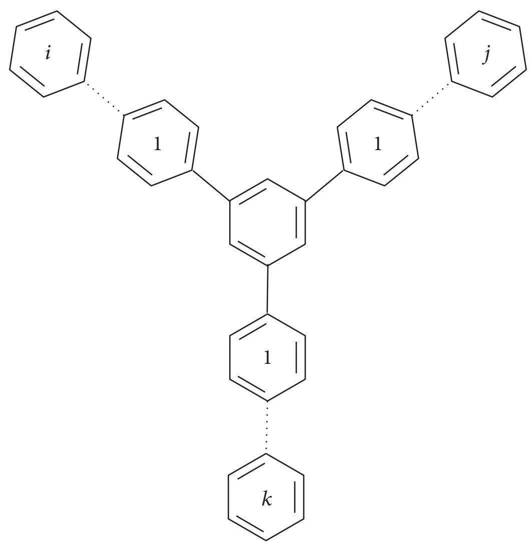

FIGURE 1: L-type polyphenyl spider.

subgraph of $l(n)$ with n hexagons obtained by deleting some vertices (see Figures 2 and 3).

We denote by Ψ_n the set of polyphenyl spiders with n hexagons. A polyphenyl spider G is called a L-type polyphenyl spider and denote $L(i, j, k)$ where $n = i + j + k + 1$ if three branches of G after deleting the hexagon which sticked by three paths P_2 are linear polyphenyl chains.

2. Some Lemmas

In this section, we will give some lemmas which will be used later.

Lemma 1 (see [1]). *Let G be a graph consisting of two components G_1 and G_2. Then*

$$Z(G) = Z(G_1)\,Z(G_2). \tag{2}$$

Lemma 2 (see [1]). *Let G be a graph and any $uv \in E(G)$. Then*

$$Z(G) = Z(G - uv) + Z(G - u - v). \tag{3}$$

By Lemmas 1 and 2, we can obtain the following two results.

Lemma 3. *Let $l(n)$ be a linear polyphenyl chain with n hexagons and $g(n)$, $h(n)$, and $q(n)$ be three chains with $n-1$ hexagons. Then*

(i) $Z(g(n)) = 8Z(l(n-1)) + 4Z(g(n-1))$,

(ii) $Z(q(n)) = 8Z(l(n-1)) + 3Z(g(n-1))$,

(iii) $Z(h(n)) = 3Z(l(n-1)) + Z(g(n-1))$.

Lemma 4. *Let $L(i, j, k)$ be a L-type polyphenyl spider with n hexagons. Then*

$$\begin{aligned} Z(L(i,j,k)) = {} & Z(l(k))\,Z(l(i))\,Z(l(j)) \\ & + Z(l(k))\,Z(g(i))\,Z(q(j)) \\ & + Z(g(k))\,Z(l(i))\,Z(q(j)) \\ & + Z(g(k))\,Z(g(i))\,Z(h(j)). \end{aligned} \tag{4}$$

Lemma 5 (see [24]). *Let $F(n)$ and $L(n)$ be a Fibonacci and Lucas sequences, respectively. Then*

(i) $F(n) = (\alpha^n - \beta^n)/\sqrt{5}$, $L(n) = \alpha^n + \beta^n$, *where* $\alpha = (1+\sqrt{5})/2$ *and* $\beta = (1-\sqrt{5})/2$,

(ii) $F(n)F(m) = (1/5)(L(n+m) - (-1)^n L(m-n))$,

(iii) $F(m)L(n) = F(n+m) - (-1)^m F(n-m) = F(m+n) + (-1)^n F(m-n)$.

Lemma 6 (see [25]). *Let $q_1, q_2, \ldots, q_t$ be all different roots of the homogeneous recursive formula $H(n) = a_1H(n-1) + a_2H(n-1) + \cdots + a_kH(n-k)$. And let e_i be the multiplicity of q_i $(i = 1, 2, \ldots, t)$. Then the general solution $H(n)$ of homogeneous recursive formula is $H(n) = H_1(n) + H_2(n) + \cdots + H_t(n)$, where $H_i(n) = (c_1 + c_2n + \cdots + c_{e_i}n^{e_i-1})q_i^n$ for $i = 1, 2, \ldots, t$.*

Lemma 7 (see [25]). *Let $H(n) = a_1H(n-1) + a_2H(n-1) + \cdots + a_kH(n-k) + \tau^n$ be the nonhomogeneous recursive formula, where $a_1, a_2, \ldots, a_k$ and τ are constants. If $f(n)$ is the general solution of homogeneous recursive formula $H(n) = a_1H(n-1) + a_2H(n-1) + \cdots + a_kH(n-k)$, then the general solution $H(n)$ of the above nonhomogeneous recursive formula can be expressed as $H(n) = d_1f(n) + d_2\tau^n$, where d_1 and d_2 are fixed constants.*

Lemma 8 (see [26]). *Let $l(n)$ be a linear polyphenyl chain with n hexagons. Then*

$$Z(l(n)) = \begin{pmatrix} 18 & 8 \end{pmatrix} \begin{pmatrix} 18 & 8 \\ 8 & 4 \end{pmatrix}^{n-2} \begin{pmatrix} 18 \\ 8 \end{pmatrix}. \tag{5}$$

Furthermore, Lemma 8 also can be expressed as another form, that is, the following lemma.

Lemma 9 (see [26]). *Let $l(n)$ be the linear polyphenyl chain with n hexagons. Then*

$$\begin{aligned} Z(l(n)) = {} & \frac{21922 + 2062\sqrt{113}}{113}\lambda_1^{n-2} \\ & + \frac{21922 - 2062\sqrt{113}}{113}\lambda_2^{n-2}. \end{aligned} \tag{6}$$

3. Main Results

Theorem 10. *Let $l(n)$ be a linear polyphenyl chain with n hexagons and $g(n)$, $h(n)$, and $q(n)$ be three chains with $n-1$ hexagons. Then*

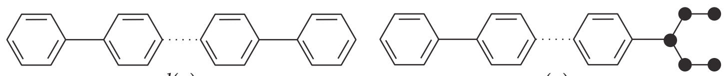

Figure 2: Chains $l(n)$ and $g(n)$.

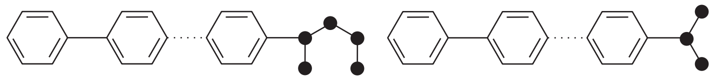

Figure 3: Chains $q(n)$ and $h(n)$.

(i) $Z(g(n)) = ((175376+16496\sqrt{113})/113(\lambda_1-4))\lambda_1^{n-2} + ((175376-16496\sqrt{113})/113(\lambda_2-4))\lambda_2^{n-2}$,

(ii) $Z(q(n)) = 8[((452226+42542\sqrt{113})/113(\lambda_1-4))\lambda_1^{n-3} + ((452226-42542\sqrt{113})/113(\lambda_2-4))\lambda_2^{n-3}]$,

(iii) $Z(h(n)) = ((1334756+125564\sqrt{113})/113(\lambda_1-4))\lambda_1^{n-3} + ((1334756-125564\sqrt{113})/113(\lambda_2-4))\lambda_2^{n-3}$.

Proof. Combining Lemmas 3 and 8 and (i) of Theorem 10, it is easy to prove (ii) and (iii) of Theorem 10. We only prove (i) of Theorem 10 as follows.

By Lemma 3, we have

$$Z(g(n)) = 8Z(l(n-1)) + 4Z(g(n-1)). \tag{7}$$

By Lemma 9, we get that

$$\begin{aligned} Z(g(n)) - 4Z(g(n-1)) &= 8\left(\frac{21922+2062\sqrt{113}}{113}\lambda_1^{n-3}\right. \\ &\quad \left. + \frac{21922-2062\sqrt{113}}{113}\lambda_2^{n-3}\right). \end{aligned} \tag{8}$$

By Lemma 6, solving the homogeneous recursive formula $Z(g(n))-4Z(g(n-1)) = 0$ of (8), we obtain that $Z(g(n)) = 4^n$. By Lemma 7, the general solution of the nonhomogeneous recursive formula (8) can be expressed as

$$\begin{aligned} Z(g(n)) = d_1 4^n + d_2 8\left(\frac{21922+2062\sqrt{113}}{113}\lambda_1^{n-3}\right. \\ \left. + \frac{21922-2062\sqrt{113}}{113}\lambda_2^{n-3}\right), \end{aligned} \tag{9}$$

where d_1 and d_2 are fixed constants. For the sake of simplicity, we set $d_3 = 8d_2((21922+2062\sqrt{113})/113)$ and $d_4 = 8d_2((21922-2062\sqrt{113})/113)$. Then the general solution of the nonhomogeneous recursive formula (9) can be expressed as

$$Z(g(n)) = d_1 4^n + d_3\lambda_1^{n-3} + d_4\lambda_2^{n-3}, \tag{10}$$

where d_1, d_3, d_4 are fixed constants. Substituting (10) into the nonhomogeneous recursive formula (8), we get that

$$\begin{aligned} d_3 &= \frac{(175376+16496\sqrt{113})\lambda_1}{113(\lambda_1-4)}, \\ d_4 &= \frac{(175376-16496\sqrt{113})\lambda_2}{113(\lambda_2-4)}, \end{aligned} \tag{11}$$

$$\begin{aligned} Z(g(n)) = d_1 4^n + \frac{(175376+16496\sqrt{113})\lambda_1}{113(\lambda_1-4)}\lambda_1^{n-3} \\ + \frac{(175376-16496\sqrt{113})\lambda_2}{113(\lambda_2-4)}\lambda_2^{n-3}. \end{aligned} \tag{12}$$

By direct calculation, we get $Z(g(4)) = 82368$. By (12), we have $d_1 = 0$. And the proof of Theorem 10 is complete. □

Theorem 11. *Let $L(i,j,k)$ be the L-type polyphenyl spider with n hexagons. Then*

$$\begin{aligned} Z(L(i,j,k)) &= \frac{(10961+1031\sqrt{113})^2(12937331+814315\sqrt{113})}{4\times 113^3} \\ &\cdot \lambda_1^{k+i+j-7} \\ &+ \frac{1024(39324+3700\sqrt{113})}{113^2}(\lambda_1^{k+j-5}\lambda_2^{i-2} + \lambda_1^{i+j-5}\lambda_2^{k-2}) \\ &+ \frac{(26150912-2455552\sqrt{113})}{113^2}\lambda_1^{j-3}\lambda_2^{k+i-4} \\ &+ \frac{(21922+2062\sqrt{113})(1995598080+186592512\sqrt{113})}{113^3} \\ &\cdot \lambda_1^{k+i-4}\lambda_2^{j-3} \\ &+ \frac{1024(39324-3700\sqrt{113})}{113^2}(\lambda_1^{k-2}\lambda_2^{i+j-5} + \lambda_1^{i-2}\lambda_2^{k+j-5}) \\ &+ \frac{(21922+2062\sqrt{113})^2(675966-63590\sqrt{113})}{113^3}\lambda_2^{k+i+j-7}. \end{aligned} \tag{13}$$

Proof. For the sake of facilitating the calculation, we set the coefficients of all formulas of Lemma 8 and Theorem 10 as follows:

$$\begin{aligned} a &= \frac{21922 + 2062\sqrt{113}}{113}, \\ b &= \frac{21922 - 2062\sqrt{113}}{113}, \\ c &= \frac{175376 + 16496\sqrt{113}}{113(\lambda_1 - 4)}, \\ d &= \frac{175376 - 16496\sqrt{113}}{113(\lambda_2 - 4)}, \\ e &= \frac{452226 + 42542\sqrt{113}}{113(\lambda_1 - 4)}, \\ w &= \frac{452226 - 42542\sqrt{113}}{113(\lambda_2 - 4)}, \\ u &= \frac{1334756 + 125564\sqrt{113}}{113(\lambda_1 - 4)}, \\ v &= \frac{1334756 - 125564\sqrt{113}}{113(\lambda_2 - 4)}. \end{aligned} \quad (14)$$

By Lemma 4, we know that

$$\begin{aligned} Z(L(i,j,k)) &= Z(l(k))Z(l(i))Z(l(j)) \\ &+ Z(l(k))Z(g(i))Z(q(j)) \\ &+ Z(g(k))Z(l(i))Z(q(j)) \\ &+ Z(g(k))Z(g(i))Z(h(j)). \end{aligned} \quad (15)$$

By Lemma 9 and Theorem 10, simplifying (15), we have

$$\begin{aligned} Z(L(i,j,k)) &= \left(a\lambda_1^{k-2} + b\lambda_2^{k-2}\right)\left(a\lambda_1^{i-2} + b\lambda_2^{i-2}\right) \\ &\cdot \left(a\lambda_1^{j-2} + b\lambda_2^{j-2}\right) + \left(a\lambda_1^{k-2} + b\lambda_2^{k-2}\right)\left(c\lambda_1^{i-2} + d\lambda_2^{i-2}\right) \\ &\cdot \left(8e\lambda_1^{j-2} + 8w\lambda_2^{j-2}\right) + \left(c\lambda_1^{k-2} + d\lambda_2^{k-2}\right)\left(a\lambda_1^{i-2} + b\lambda_2^{i-2}\right) \\ &\cdot \left(8e\lambda_1^{j-2} + 8w\lambda_2^{j-2}\right) + \left(c\lambda_1^{k-2} + d\lambda_2^{k-2}\right)\left(c\lambda_1^{i-2} + d\lambda_2^{i-2}\right) \\ &\cdot \left(u\lambda_1^{j-2} + v\lambda_2^{j-2}\right) = \left(a^3\lambda_1 + 16ace + c^2u\right)\lambda_1^{k+i+j-7} \\ &+ \left(b^2a\lambda_1 + 16bde + d^2u\right)\lambda_1^{j-3}\lambda_2^{k+i-4} \\ &+ \left(a^2b\lambda_1 + 8ade + 8bce + cdu\right)\left(\lambda_1^{k+j-5}\lambda_2^{i-2} + \lambda_1^{i+j-5}\lambda_2^{k-2}\right) \\ &+ \left(ab^2\lambda_2 + 8adw + 8bcw + cdv\right)\left(\lambda_1^{k-2}\lambda_2^{i+j-5} + \lambda_1^{i-2}\lambda_2^{k+j-5}\right) \\ &+ \left(a^2b\lambda_2 + 8adw + 8bcw + c^2v\right)\lambda_1^{k+i-4}\lambda_2^{j-3} \\ &+ \left(b^3\lambda_2 + 16bdw + d^2v\right)\lambda_2^{k+i+j-7} \\ &= \frac{\left(10961 + 1031\sqrt{113}\right)^2\left(12937331 + 814315\sqrt{113}\right)}{4 \times 113^3} \\ &\cdot \lambda_1^{k+i+j-7} \\ &+ \frac{1024\left(39324 + 3700\sqrt{113}\right)}{113^2}\left(\lambda_1^{k+j-5}\lambda_2^{i-2} + \lambda_1^{i+j-5}\lambda_2^{k-2}\right) \\ &+ \frac{\left(26150912 - 2455552\sqrt{113}\right)}{113^2}\lambda_1^{j-3}\lambda_2^{k+i-4} \\ &+ \frac{\left(21922 + 2062\sqrt{113}\right)\left(1995598080 + 186592512\sqrt{113}\right)}{113^3} \\ &\cdot \lambda_1^{k+i-4}\lambda_2^{j-3} \\ &+ \frac{1024\left(39324 - 3700\sqrt{113}\right)}{113^2}\left(\lambda_1^{k-2}\lambda_2^{i+j-5} + \lambda_1^{i-2}\lambda_2^{k+j-5}\right) \\ &+ \frac{\left(21922 + 2062\sqrt{113}\right)^2\left(675966 - 63590\sqrt{113}\right)}{113^3}\lambda_2^{k+i+j-7}. \end{aligned} \quad (16)$$

□

By Theorem 11, we can obtain two corollaries as follows.

Corollary 12. *Let $L(i, j, k)$ be a L-type polyphenyl spider with n hexagons. Then*

$$Z(L(i,j,k)) \ge \begin{cases} Z\left(L\left(\frac{n-1}{3}, \frac{n-1}{3}, \frac{n-1}{3}\right)\right) & 0 \bmod (3), \\ Z\left(L\left(\frac{n-2}{3}, \frac{n-2}{3}, \frac{n+1}{3}\right)\right) & 1 \bmod (3), \\ Z\left(L\left(\frac{n-3}{3}, \frac{n}{3}, \frac{n}{3}\right)\right) & 2 \bmod (3). \end{cases} \quad (17)$$

Particularly, the equality holds if and only if

$$Z(L(i,j,k)) \cong \begin{cases} Z\left(L\left(\frac{n-1}{3}, \frac{n-1}{3}, \frac{n-1}{3}\right)\right) & 0 \bmod (3), \\ Z\left(L\left(\frac{n-2}{3}, \frac{n-2}{3}, \frac{n+1}{3}\right)\right) & 1 \bmod (3), \\ Z\left(L\left(\frac{n-3}{3}, \frac{n}{3}, \frac{n}{3}\right)\right) & 2 \bmod (3). \end{cases} \quad (18)$$

Corollary 13. *Let $L(i, j, k)$ be the L-type polyphenyl spider with n hexagons. Then*

$$Z(L(i,j,k)) \le Z(L(1,1,n-3)), \quad (19)$$

where the equality holds if and only if $Z(L(i,j,k)) \cong Z(L(1,1,n-3))$.

4. Conclusion

In this paper, applying the relation between inhomogeneous constant coefficient recursion formula and constant coefficient recursion formula, we give a computing formula of Hosoya index of a L-type polyphenyl spider. Furthermore, we determine completely the L-type polyphenyl spider which has the largest and smallest Hosoya index.

Competing Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgments

This work is supported by NSFC (11502132), NSF of Qinghai (2016-ZJ-947Q), education department of Shaanxi province (15JK1135), and Shaanxi Sci-Tech University (SLGQD14-14).

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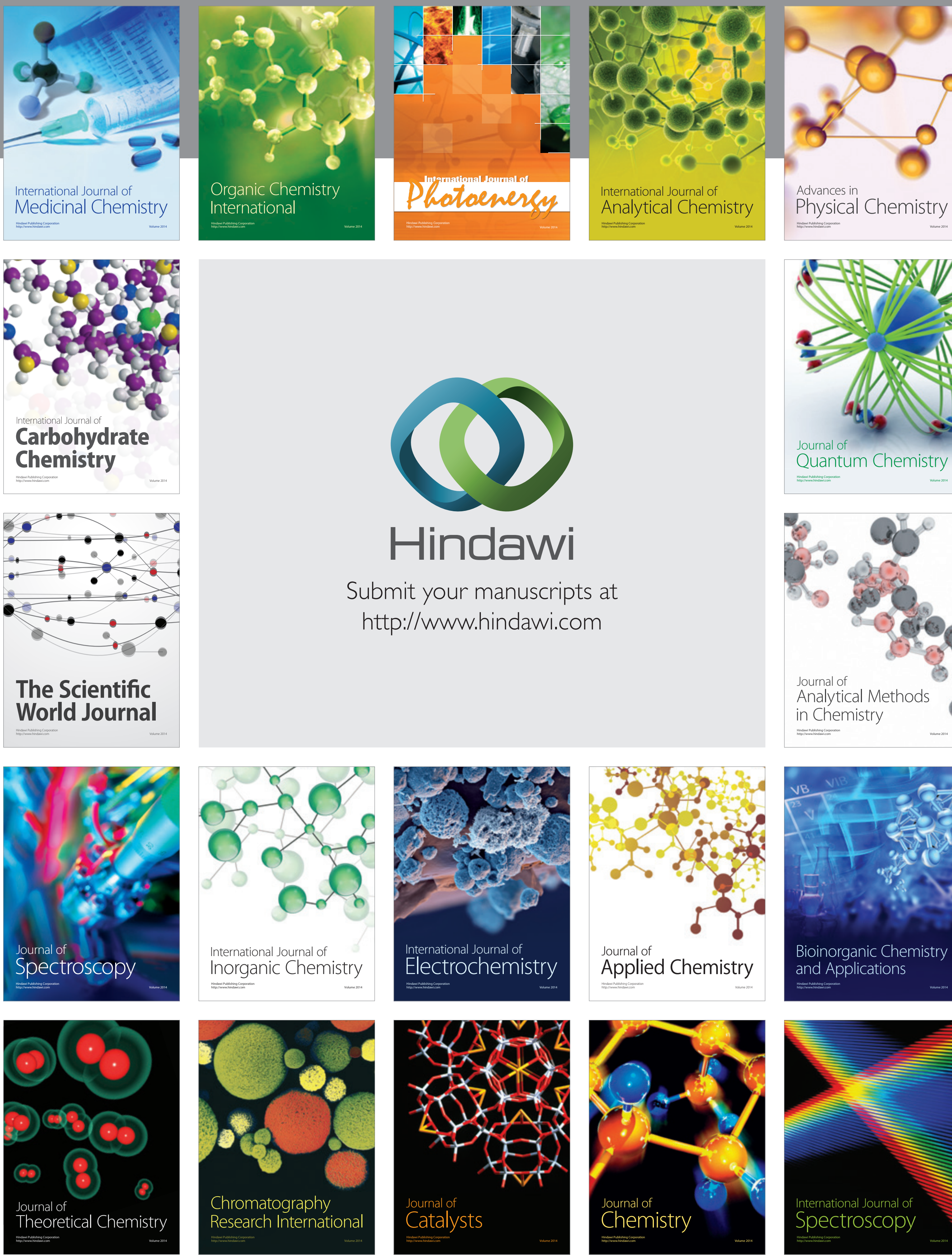
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