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Applications of graph operations

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ABSTRACT

In this paper, some applications of our earlier results in working with chemical graphs are presented.

Keywords: Topological index, graph operation, hierarchical product, chemical graph.

1. INTRODUCTION

Throughout this paper all graphs considered are finite, simple and connected. The distance $d_G(u,v)$ between the vertices u and v of a graph G is equal to the length of a shortest path that connects u and v. Suppose G is a graph with vertex and edge sets $V = V(G)$ and $E = E(G)$, respectively, and $e = ab \in E(G)$. The set of edges of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $M_u^G(e)$. Then the edge PI index of G, $PI_e(G)$, is defined as $PI_e(G) = \sum_{e=uv\in E(G)} \left(\left|M_u^G(e)\right| + \left|M_v^G(e)\right| \right)$ [1,2]. In a similar way, $N_a^G(e)$ is defined as the set of vertices closer to the vertex a than to the vertex b. In other words, $N_a^G(e) = \{u \in V(G) \mid d(u, a) < d(u, b)\}$. The vertex PI index of G, $PI_v(G)$, is defined as $[|N_u^G(e)| + |N_v^G(e)|]$ over all edges of G [3,4]. The edges $e = uv$ and $f = xy$ of G are said to be equidistant if $min\{d_G(u, x), d_G(u, y)\} = min\{d_G(v, x), d_G(v, y)\}$. For $e = uv \in G$, the set

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of equidistant vertices of e is denoted by $N_0^G(e)$ and the set of equidistant edges of e is denoted by $M_0^G(e)$. Then the above definitions are equivalent to

$$PI_v(G) = |V(G)||E(G)| - \sum_{e\in E(G)} \left|N_0^G(e)\right|,$$

$$PI_e(G) = |E(G)|^2 - \sum_{e\in E(G)} \left|M_0^G(e)\right|.$$

A graph G with a specified vertex subset $U \subseteq V(G)$ is denoted by $G(U)$. Suppose G and H are graphs and $U \subseteq V(G)$. The generalized hierarchical product, denoted by $G(U)\Pi H$, is the graph with vertex set $V(G)\times V(H)$ and two vertices (g, h) and (g', h') are adjacent if and only if $g = g' \in U$ and $hh' \in E(H)$ or, $gg' \in E(G)$ and $h = h'$. This graph operation has been introduced by Barriére et al. [5,6] and it has some applications in computer science. To generalize this graph operation to n graphs, assume that $G_i = (V_i , E_i)$ is a graph with vertex set V_i , $1 \le i \le N$, having a distinguished or root vertex 0. The hierarchical product $H = G_N \Pi \ldots \Pi G_2 \Pi G_1$ is the graph with vertices the N–tuples $x_N \ldots x_3x_2x_1$, $x_i \in V_i$, and edges defined by the following adjacencies:

$$x_N \ldots x_3x_2x_1 \sim \begin{cases} x_N \ldots x_3x_2y_1 & \text{if} \quad x_1y_1 \in E(G_1), \\ x_N \ldots x_3y_2x_1 & \text{if} \quad x_2y_2 \in E(G_2) \text{ and } x_1 = 0, \\ x_N \ldots y_3x_2x_1 & \text{if} \quad x_3y_3 \in E(G_3) \text{ and } x_1 = x_2 = 0, \\ \vdots & \vdots \qquad\qquad\qquad\qquad \vdots \\ y_N \ldots x_3x_2x_1 & \text{if} \quad x_Ny_N \in E(G_N) \text{ and } x_1 = x_2 = \ldots = x_{N-1} = 0. \end{cases}$$

We encourage the reader to consult [7] for the mathematical properties of the hierarchical product of graphs.

2. MAIN RESULTS

Let $G = (V, E)$ be a graph and $U \subseteq V$. Following Pattabiraman and Paulraja [8], an u–v path through U in $G(U)$ is an u–v path in G containing some vertex $w \in U$ (not necessarily distinct from the vertices u and v). Let $d_{G(U)}(u,v)$ denote the length of a shortest u–v path through U in G. Notice that, if one of the vertices u and v belong to U, then $d_{G(U)}(u,v) = d_G(u,v)$. A vertex $x \in V(G(U))$ is said to be equidistant from $e = uv \in E(G(U))$ through U in $G(U)$, if $d_{G(U)}(u, x) = d_{G(U)}(v, x)$. For an edge $e = ab$ in $G(U)$, let $N_0^{G(U)}(e)$ denote the set of equidistant vertices of e through U in $G(U)$ and $N_a^{G(U)}(e)$ denote the set of vertices closer to a than to b through U in G. Then $PI_v(G(U))$ and $PI_e(G(U))$ can be computed by the following formula:

$$PI_v(G(U)) = \sum_{e=ab\in E(G(U))}\left(\left|N_a^{G(U)}(e)\right| + \left|N_b^{G(U)}(e)\right|\right)$$
$$= |V(G(U))||E(G(U))| - \sum_{e\in E(G(U))}\left|N_0^{G(U)}(e)\right|.$$

The edges $e = uv$ and $f = xy$ of $G(U)$ are said to be equidistant edges through U in $G(U)$ if

$$min\{d_{G(U)}(u, x), d_{G(U)}(u, y)\} = min\{d_{G(U)}(v, x), d_{G(U)}(v, y)\}.$$

Let $M_0^{G(U)}(e)$ denote the set of equidistant edges of e through U in $G(U)$ and $M_a^{G(U)}(e)$ denote the set of edges closer to a than to b through U in G. Then $PI_e(G(U))$ is computed as follows:

$$PI_v(G(U)) = \sum_{e=ab\in E(G(U))}\left(\left|M_a^{G(U)}(e)\right| + \left|M_b^{G(U)}(e)\right|\right)$$
$$= |E(G(U))|^2 - \sum_{e\in E(G(U))}\left|M_0^{G(U)}(e)\right|.$$

Theorem 1. [9]. Let G and H be two connected graphs and let U be a nonempty subset of $V(G)$. Then $PI_v(G(U) \Pi H) = |V(H)| (|V(H)| - 1) PI_v(G(U)) + |V(H)|PI_v(G) + |V(G)||U|PI_v(H)$.

Theorem 2. [9]. Let G and H be two connected graphs and let U be a nonempty subset of $V(G)$. Then

$$PI_e(G(U) \Pi H) = |V(H)|(|V(H)| - 1)PI_e(G(U)) + |V(H)|PI_e(G)$$
$$+ |V(H)||E(H)|\Big(|U||E(G)| - \sum_{gg'\in E(G(U))}\left|N_0^{G(U)}(gg')\cap U\right|\Big)$$
$$+ |E(G)||U|PI_v(H) + |U|^2PI_e(H).$$

We are now ready to obtain the PI indices of some chemical graphs.

Example 3. Let H be the graph of truncated cuboctahedron (see Figure 1). Then $H = ((P_6(U_1) \Pi P_2)(U_2) \Pi P_2)(U3) \Pi P_2$, where $U_1 = \{1, 2, 5, 6\}$, $U_2 = \{7, 9, 10, 12\}$ and $U_3 = \{1, 3, 4, 6, 19, 21, 22, 24\}$. One can see that $PI_e(P_6(U_1) \Pi P_2) = 2\times 20 + 2\times 20 + 2\times (4\times 5) + 5\times 4\times 2 = 160$. Also $PI_e((P_6(U_1) \Pi P_2)(U_2) \Pi P_2) = 2\times 176 + 2\times 160 + 2\times 4\times 14 + 14\times 4\times 2 = 896$. Thus, by Theorem 1, we have

$$PI_e(H) = 2\times 896 + 2\times 896 + 2\times 8\times 32 + 32\times 8\times 2 = 4608.$$

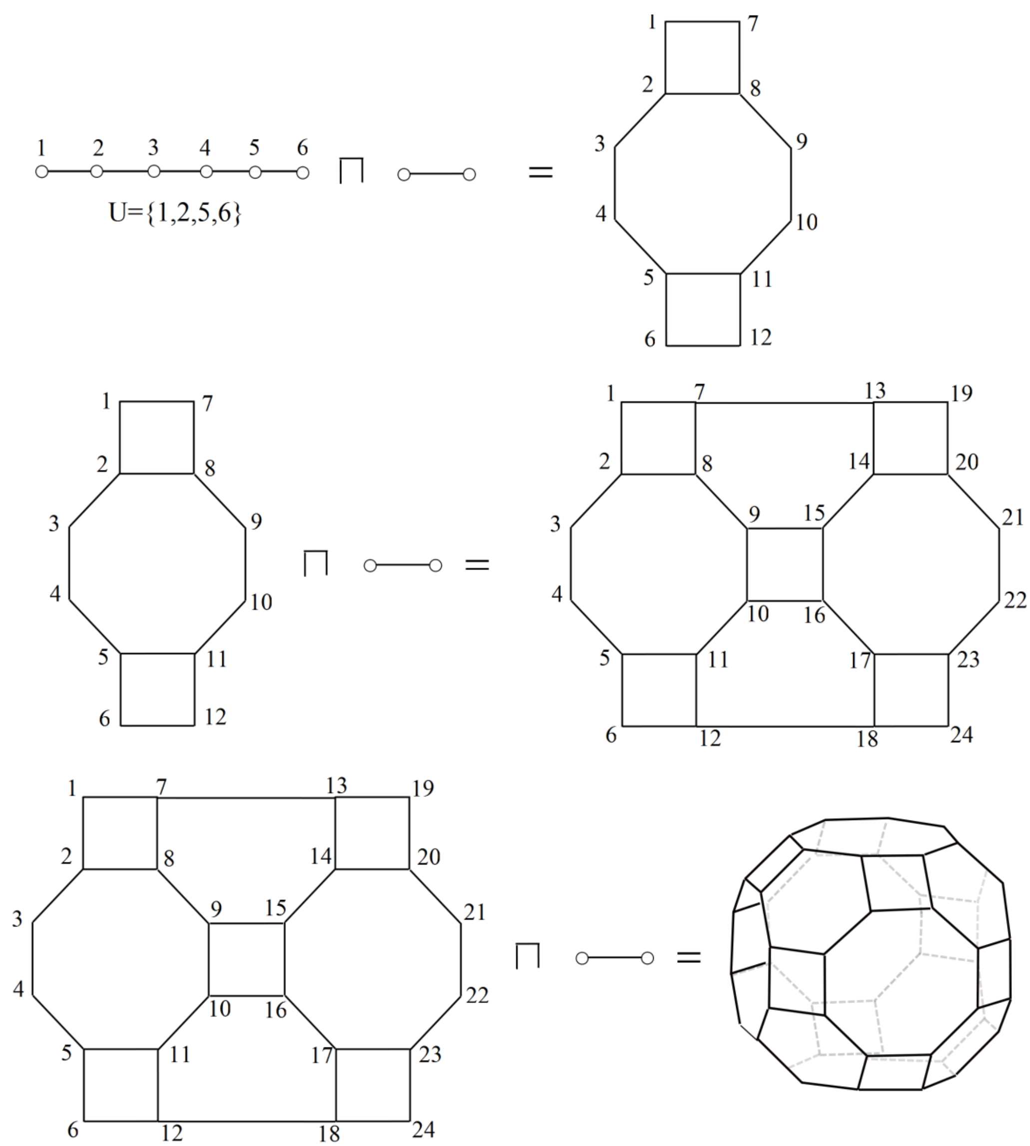

Figure 1. The Molecular Graph of Truncated Cuboctahedron.

Example 4. Octanitrocubane is the most powerful chemical explosive with formula $C_8(NO_2)_8$), part (a) of Fig. 2. Let H be the molecular graph of this molecule. Then obviously $H= P_4(U) \Pi Q_2$, where $U = \{2, 3\}$. On the other hand, one can easily see that $PI_e(P_4(U))=8$ and $PI_e(P_4) = 6$ and so, by Theorem 1, we have

$$PI_e(P_4(U) \Pi Q_2) = 4 \times 3 \times 8 + 4 \times 6 + 4 \times 4 \times (2 \times 3) + 3 \times 2 \times 16 + 4 \times 8 = 344.$$

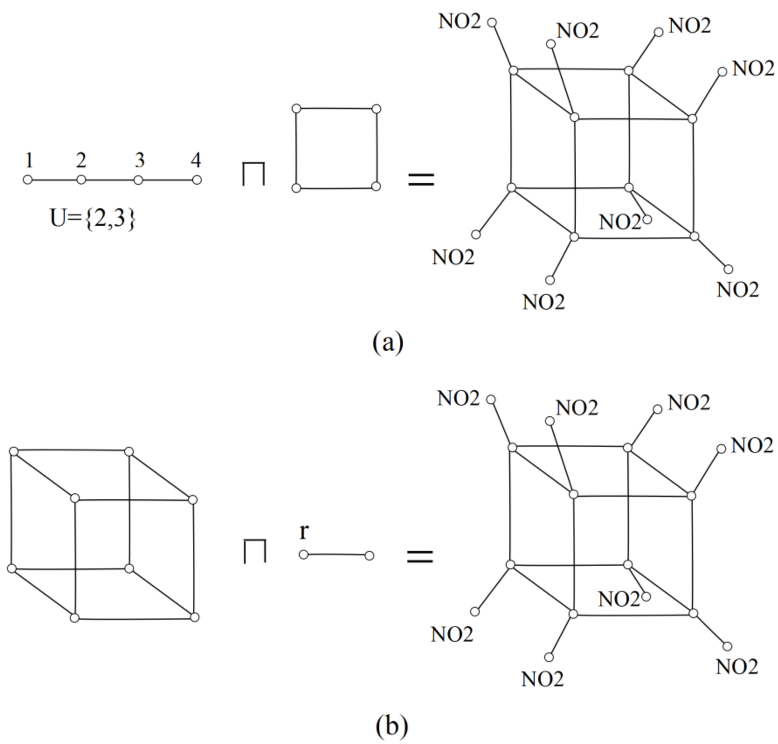

Figure 2. The Molecular Graph of Octanitrocubane.

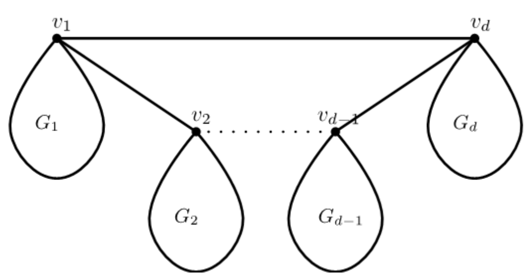

Figure 3. The Bridge−Cycle Graph.

Example 5. Let $\{G_i\}_{i=1}^{d}$ be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$. The bridge−cycle graph $BC(G_1, G_2, \ldots, G_d) = BC(G_1, G_2, \ldots, G_d; v_1, v_2, \ldots, v_d)$ of $\{G_i\}_{i=1}^{d}$ with respect to the vertices $\{v_i\}_{i=1}^{d}$ is the graph obtained from the graphs $G_1, \ldots, G_d$ by connecting the vertices v_i and v_{i+1} by an edge for all $i = 1, 2, \ldots, d-1$ and connecting the vertices v_1 and v_d by an edge, see Fig. 3. Suppose that $G_1 = \ldots = G_d = G$. Then we have

$BC(G_1, G_2, \ldots, G_d) \cong G(U)\Pi\, C_d$, where $|U|=|\{r\}|=1$. On the other hand, It is not so difficult to check that $PI_e(C_n)=\begin{cases} n(n-1) & 2\nmid n \\ n(n-2) & 2\mid n \end{cases}$ and $PI_v(C_n)=\begin{cases} n(n-1) & 2\nmid n \\ n^2 & 2\mid n \end{cases}$. Therefore, if $2 \mid m$, by Theorem 1, we have $PI_e(G(U)\Pi C_m) = m(m-1)PI_e(G(U)) + mPI_e(G) + m^2(2|E(G)| - N_r(G)) + m(m-2)$ and if $2 \nmid m$, then $PI_e(G(U)\Pi C_m) = m(m-1)PI_e(G(U)) + mPI_e(G) + m^2(2|E(G)| - N_r(G)) - m|E(G)| + m(m-1)$, where $N_r(G)=|\{uv\in E(G) \mid d_G(u,r)=d_G(v,r)\}|$.

By replacing G with P_n (such that r is a pendant vertex of P_n) in the above relations, we obtain PI_e of $Sun_{m,\, n-1}$, see [10], as follow:

$$PI_e(Sun_{m,\, n-1})=\begin{cases} m^2n^2-2mn+m & 2\nmid m \\ m^2n^2-mn-m & 2\mid m \end{cases}.$$

In what follows, let $\prod_i^j f_i = 1$ and $\sum_i^j f_i = 0$ for each $i, j \in \{0, 1, 2, \ldots\}$, that $i-j = 1$. Furthermore, let $\prod_i^j f_i = \sum_i^j f_i = 0$ for every $i, j \in \{0, 1, 2, \ldots\}$, such that $i-j > 1$. Also, for a sequence of graphs, $G_1, G_2, \ldots, G_n$, we set $|V_{i,j}| = \prod_{k=i}^j |V(G_k)|$ and $|V_{i,j}^l| = \prod_{k=i,k\neq l}^j |V(G_k)|$.

Theorem 6. [11]. Suppose $G_1, G_2, \ldots, G_n$ are connected rooted graphs with root vertices $r_1, \ldots, r_n$, respectively. Then

$$\begin{aligned} PI_e(G_n\Pi \ldots \Pi G_2\Pi G_1) &= \sum_{i=1}^n |V_{i+1,n}| PI_e(G_i) + \sum_{i=1}^n |V_{i+1,n}| \left(\sum_{j=1}^{i-1} |E(G_j)||V_{j+1,i-1}| \right) PI_v(G_i) \\ &+ \sum_{i=1}^n ((|E(G_i)| - N_{r_i})|V_{i+1,n}| \sum_{j=i+1}^n ((|V(G_j)|-1) \\ &= \sum_{k=1}^{j-1} |E(G_k)||V_{k+1,j-1}| + |E(G_j)|)), \end{aligned}$$

where $N_{r_i} = |\{uv\in E(G_i) \mid d_{G_i}(u,r_i) = d_{G_i}(v,r_i)\}|$.

Example 7. Let Γ be the graph of octanitrocubane, see part (b) of Figure 6. Then obviously $H= Q_3\, \Pi\, P_2$. On the other hand, one can easily see that $PI_e(Q_3) = PI_v(Q_3) = 96$ and $PI_e(P_2) = 0$ and so, by Theorems 6, we have $PI_e(P_6(U)\Pi Q_2) = 344$.

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