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EDGE VERSION OF NEW JOIN GRAPHS AND THEIR INVARIANT

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Abstract: A molecular structure descriptor(topological descriptor) is numerical value associated with chemical construction for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. The topological descriptors are very important role in mathematical chemistry, especially, they are used in the studies of $QSAR/QSPR$. In this paper, we study the H-invariant of edge version of new join graphs.

Keywords and Phrases: Graph invariant, Degree, Topological descriptor.

2010 Mathematics Subject Classification: 05C12, 05C76.

1. Introduction and Preliminaries

Quantitative structure-activity relationship models (QSAR models) are regression or classification models used in the chemical and biological sciences and control system engineering. One of the first historical QSAR chemical applications was to predict boiling points. Those numerical quantities which transform a chemical structure to a numerical number called the topological descriptors/indices. In QSAR study, chemical graph theory plays an important role in modelling of organic chemical structures to hydrogen depleted graphs in which vertices correspond to atoms and edges correspond the bonds in the underlying chemical compounds.

The Zagreb invariants have been introduced more than thirty years ago by Gutman and Trinajestić [4]. They are defined as $M_1(G) = \sum\limits_{uv \in E(G)} (d_G(u) + d_G(v))$

and $M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)$. The Zagreb invariants are found to have applications in QSPR and QSAR studies as well. Furtula and Gutman in [3] recently investigated this invariant and named this invariant as F-invariant and showed that the predictive ability of this invariant is almost similar to that of first Zagreb invariant and for the entropy and acetic factor, both of them yield correlation coefficients greater than 0.95. The F-invariant of a graph G is defined as $F(G) = \sum_{u\in V(G)} d_G^3(u) = \sum_{uv\in E(G)} (d_G^2(u) + d_G^2(v))$.

Recently, Shirdel et al. [6] introduced a variant of the first Zagreb invariant called H-invariant which defined as $HZ(G) = \sum_{uv\in E(G)} (d(u)+d(v))^2$. For the survey on theory and application of Zagreb indices see [5]. Feng et al. [1] have given a sharp bounds for the Zagreb invariants of graphs with a given matching number. Some upper and lower bounds on H-invariant for a connected graph are obtained by Falahati-Nezhad and Azari [2]. In this paper, we study the H-invariant for a new product of graphs based on join operation.

2. H-invariant of graphs

Let G be a connected graph. The subdivision graph $S(G)$ is the graph obtained from G by replacing each edge of G by a path of length two. The edge S-join graph of two graphs G_1 and G_2 denoted by $G_1 \vee_s G_2$ and is obtained from $S(G_1)$ and G_2 by joining each vertex of $I(G_1)$ with every vertex of G_2. The graph $R(G)$ is obtained from G by adding a new vertex corresponding to each edge of G, then joining each new vertex to the end vertices of the corresponding edge. The edge R-join graph of two graphs G_1 and G_2 denoted by $G_1 \vee_R G_2$ and is obtained from $R(G_1)$ and G_2 by joining each vertex of $I(G_1)$ with every vertex of G_2.

Theorem 2.1. *Let G_i be (n_i, m_i) graph, $i = 1, 2$. Then* $HZ(G_1 \vee_s G_2) = F(G_1) + HZ(G_2) + 5m_1M_1(G_2) + 2(n_2+2)M_1(G_1) + 2m_1(n_2+2)^2 + 4{m_1}^2m_2 + (n_2+m_1+2)^2m_1n_2 + 4(n_2+m_1+2)m_1m_2$.

Proof. From the definition of edge version of S-join graph, the degree of a vertex $v \in G_1 \vee_S G_2$ is given by $d_{G_1\vee_S G_2}(v) = \begin{cases} d_{G_1}(v), \text{if} \quad v\in V(G_1) \\ 2+n_2, \text{if} \quad v \in I(G_1) \\ d_{G_2}(v)+m_2, \text{if} \quad v\in V(G_2). \end{cases}$

Hence $HZ(G_1 \vee_s G_2) = \sum_{xy\in E(G_1\vee_s G_2)} \Big(d_{G_1\vee_s G_2}(x) + d_{G_1\vee_s G_2}(y)\Big)^2$.

$$HZ(G_1 \vee_s G_2) = \sum_{xy\in E(S(G_1))} \Big(d_{G_1\vee_s G_2}(x) + d_{G_1\vee_s G_2}(y)\Big)^2$$

$$+ \sum_{xy\in E(G_2)} \Big(d_{G_1\vee_s G_2}(x)+d_{G_1\vee_s G_2}(y)\Big)^2 + \sum_{x\in I(G_2),y\in V(G_2)} \Big(d_{G_1\vee_s G_2}(x)+d_{G_1\vee_s G_2}(y)\Big)^2$$
$$= \sum_{xy\in E(S(G_1))} (d_{G_1}(y)+n_2+2)^2 + \sum_{xy\in E(G_2)} (d_{G_2}(x)+n_1+d_{G_2}(y)+m_1)^2$$
$$+ \sum_{x\in I(G_1),y\in V(G_2)} (2+n_2+d_{G_2}(y)+m_1)^2$$
$$= \sum_{y\in V(G_1)} d_{G_1}(y)\Big(d^2_{G_1}(y)+(n_2+2)^2+2(n_2+2)d_{G_1}(y)\Big)$$
$$+ \sum_{xy\in E(G_2)} \Big((d_{G_2})(x)+d_{G_2}(y))^2+4m_1^2+4m_1(d_{G_2}(x)+d_{G_2}(y))\Big)$$
$$+ m_1 \sum_{y\in V(G_2)} \Big(d^2_{G_2}(y)+(n_2+m_1+2)^2+2(n_2+m_1+2)d_{G_2}(y)\Big)$$
$$= F(G_1)+HZ(G_2)+5m_1M_1(G_2)+2(n_2+2)M_1(G_1)+2m_1(n_2+2)^2+4{m_1}^2m_2$$
$$+ (n_2+m_1+2)^2m_1n_2+4(n_2+m_1+2)m_1m_2.$$

The graph $R(G)$ is obtained from G by adding a new vertex corresponding to each edge of G, then joining each new vertex to the end vertices of the corresponding edge. The edge R-join graph of two graphs G_1 and G_2 denoted by $G_1 \vee_R G_2$ and is obtained from $R(G_1)$ and G_2 by joining each vertex of $I(G_1)$ with every vertex of G_2.

Theorem 2.2. *Let G_i be (n_i, m_i) graph, $i = 1, 2$. Then $HZ(G_1\vee_R G_2) = 4HZ(G_1)+HZ(G_2)+9M_1(G_1)(n_2+2)+(4m_1+1)M_1(G_2)+(m_2(n_2+2)+m_1)^2n_2+4m_2(m_2(n_2+2)+m_1)+4m_1^2m_2$.*

Proof. From the definition of edge version of R-join graph, the degree of a vertex $v \in G_1 \vee_R G_2$ is given by $d_{G_1\vee_R G_2}(y) = \begin{cases} 2d_{G_1}(y), \text{if} & y\in V(G_1)\\ 2+n_2, \text{if} & y\in I(G_1)\\ d_{G_2}(y)+m_1, \text{if} & y\in V(G_2)\end{cases}$ From the definition of H invariant, we have

$$HZ(G_1\vee_R G_2) = \sum_{xy\in E(G_1\vee_R G_2)} \Big(d_{G_1\vee_R G_2}(x)+d_{G_1\vee_R G_2}(y)\Big)^2$$
$$= \Big[\sum_{xy\in E(G_1)} + \sum_{x\in I(G_1),y\in V(G_1)} + \sum_{x\in I(G_1),y\in V(G_2)} + \sum_{xy\in E(G_2)}\Big]\Big(d_{G_1\vee_R G_2}(x)+d_{G_1\vee_R G_2}(y)\Big)^2$$
$$= \sum_{xy\in E(G_1)} (2d_{G_1}(x)+2d_{G_1}(y))^2 + \sum_{x\in I(G_1),y\in V(G_1)} (d_{I(G_1)}(x)+2d_{I(G_1)}(y))^2$$
$$+ \sum_{y\in V(G_2)} (m_2(n_2+2)+d_{G_2}(y)+m_1)^2 + \sum_{xy\in E(G_2)} (d_{G_2}(x)+m_1+d_{G_2}(y)+m_1)^2$$

$$\begin{aligned}
&= 4HZ(G_1) + (n_2+2) \sum_{y \in V(G_1)} (3d_{G_1}(y))^2 \\
&+ \sum_{y \in V(G_2)} \Big((m_2(n_2+2)+m_1)^2 + d_{G_2}^2(y) + 2d_{G_2}(y)(m_2(n_2+2)+m_1) \Big) \\
&+ \sum_{xy \in E(G_2)} \Big((d_{G_2}(x)+d_{G_2}(y))^2 + 4m_1^2 + 4m_1(d_{G_2}(x)+d_{G_2}(y)) \Big) \\
&= 4HZ(G_1) + HZ(G_2) + 9M_1(G_1)(n_2+2) + (4m_1+1)M_1(G_2) \\
&+ (m_2(n_2+2)+m_1)^2 n_2 + 4m_2(m_2(n_2+2)+m_1) + 4m_1^2 m_2.
\end{aligned}$$

The graph $Q(G)$ is obtained from G by inserting a new vertex into each edge of G, then joining with edges those pairs of new vertices on adjacent edges of G. The edge Q-join graph of two graphs G_1 and G_2 denoted by $G_1 \vee_Q G_2$ and is obtained from $Q(G_1)$ and G_2 by joining each vertex of $I(G_1)$ with every vertex of G_2.

Theorem 2.3. *Let G_i be (n_i, m_i) graph, $i = 1, 2$. Then* $HZ(G_1 \vee_Q G_2) = HZ(L(G_1)) + n_2 HZ(G_2) + 4HZ(G_1) + \Big(2(n_2+2)^2 - 16(n_2+2) + 4n_2 + 4m_2 + 2n_2(m_1+n_2)\Big) M_1(G_1) + 5m_1 M_1(G_2) + 4(n_2+2)(F(G_1) + 2M_2(G_1)) + M_1(4m_1m_2 + n_2(m_1+n_2)^2 - 3n_2^2 + 16)$.

Proof. By the definition of edge version of Q-join graph, the degree of a vertex $v \in G_1 \vee_Q G_2$ is given by $d_{G_1 \vee_Q G_2}(y) = \begin{cases} d_{G_1}(y), \text{if} \quad y \in V(G_1) \\ d_{G_2}(y) + m_1, \text{if} \quad y \in V(G_2) \\ d_{G_1}(u) + d_{G_1}(v) + n_2, \text{if} \quad e = uv, e \in I(G_1). \end{cases}$

Thus $HZ(G_1 \vee_Q G_2) = \sum_{xy \in E(G_1 \vee_Q G_2)} \Big(d_{G_1 \vee_Q G_2}(x) + d_{G_1 \vee_Q G_2}(y) \Big)^2 = I_1 + I_2 + I_3 + I_4$, where

$$\begin{aligned}
I_1 &= \sum_{xy, yu \in E(G_1)} (d_{G_1}(x) + d_{G_1}(y) + n_2 + d_{G_1}(y) + d_{G_1}(u) + n_2)^2 \\
&= \sum_{e,f \in L(G_1), e=xy, f=yu} \Big(d_{L(G_1)}(e) + 2 + n_2 + d_{L(G_1)}(f) + 2 + n_2 \Big)^2 \\
&= \sum \Big[(d_{L(G_1)}(e) + d_{L(G_1)}(f))^2 + 4(n_2+2)(d_{L(G_1)}(e) + d_{L(G_1)}(f)) + 4(n_2+2)^2 \Big] \\
&= HZ(L(G_1)) + 4(n_2+2)M_1(L(G_1)) + 4(n_2+2)^2 \left| E(L(G_1)) \right| \\
&= HZ(L(G_1)) + 4(n_2+2)\Big(F(G_1) - 4M_1(G_1) + 2M_2(G_1) + 4m_1 \Big) \\
&\quad + 4(n_2+2)^2 \Big(\frac{M_1(G_1)}{2} - m_1 \Big).
\end{aligned}$$

$I_2 = \sum_{xy \in E(G_1)} (d_{G_1}(x) + 2d_{G_1(y)} + d_{G_1}(x) + d_{G_1}(y) + n_2)^2 = 4HZ(G_1) + n_2^2 m_1 + 4M_1(G_1)n_2$.

$I_3 = \sum_{y\in V(G_2)} \sum_{x\in I(G_1)} (d_{I(G_1)}(x) + n_2 + d_{G_2}(y) + m_1)^2 = n_2HZ(G_2) + m_1M_1(G_2) + (n_2 + m_1)^2 n_2 m_1 + M_1(G_1)4m_2 + 2(n_2 + m_1)^2 M_1(G_1)n_2 + 2(n_2 + m_1)^2 m_1 M_1(G_2)$.

$I_4 = \sum_{xy\in E(G_2)} (d_{G_2}(x) + m_1 + d_{G_2}(y) + m_1)^2 = HZ(G_2) + 4m_1^2 m_2 + 4m_1M_1(G_2)$.

Adding I_1 to I_4, we obtain the required result.

The total graph $T(G)$ has as its vertices the edges and vertices of G. Adjacency in $T(G)$ is defined as adjacency or incidence for the corresponding elements of G. The edge T-join graph of two graphs G_1 and G_2 denoted by $G_1 \vee_T G_2$ and is obtained from $T(G_1)$ and G_2 by joining each vertex of $I(G_1)$ with every vertex of G_2.

Theorem 2.4. *Let G_i be (n_i, m_i) graph, $i = 1, 2$. Then* $HZ(G_1\vee_T G_2) = HZ(L(G_1)) + HZ(G_1)(n_2 + 13) + HZ(G_2) + M_1(G_1)\Big(4m_2 + 4n_2^2 + 2n_2(m_1 - 1)\Big) + 5m_1M_1(G_1) + 4(n_2 + 2)\Big(F(G_1) + 2m_2(G_2)\Big) + m_1(n_2 + m_1)\Big((n_2 + m_1)n_2 + 4m_2\Big) + 4m_1(m_1m_2 - (n_2^2 - 4)) + n_2^2 m_1$.

Proof. By the definition of edge version of Q-join graph, the degree of a vertex $v \in G_1\vee_T G_2$ is given by $d_{G_1\vee_T G_2}(y) = \begin{cases} 2d_{G_1}(y), \text{if} \quad y \in V(G_1) \\ d_{G_2}(y) + m_1, \text{if} \quad y \in V(G_2) \\ d_{G_1}(u) + d_{G_1}(v) + n_2, \text{if} \quad e = uv, e \in I(G_1). \end{cases}$

Hence $HZ(G_1\vee_T G_2) = \sum_{xy\in E(G_1\vee_T G_2)} \Big(d_{G_1\vee_T G_2}(x) + d_{G_1\vee_T G_2}(y)\Big)^2 = I_1 + I_2 + I_3 + I_4 + I_5,$ where

$I_1 = \sum_{xy\in E(I(G_1))} \Big(d_{I(G_1)}(x) + d_{I(G_1)}(y)\Big)^2 = HZ(L(G_1)) + 4(n_2 + 2)\Big(F(G_1) - 4M_1(G_1) + 2M_2(G_1) + 4m_1\Big) + 4(n_2 + 2)^2\Big(\frac{M_1(G_1)}{2} - m_1\Big)$.

$I_2 = \sum_{x\in V(G_1), y\in I(G_1)} (d_{G_1}(x) + d_{I(G_1)}(y))^2 = \sum_{xy\in E(G_1)} \Big(2d_{G_1}(x) + 2d_{G_1}(y) + d_{G_1}(x) + d_{G_1}(y) + n_2\Big)^2 = 9HZ(G_1) + n_2^2 m_1 + 6M_1(G_1)n_2$.

$I_3 = \sum_{x\in I(G_1), y\in V(G_2)} (d_{I(G_1)}(x) + n_2 + d_{G_2}(y) + m_1)^2 = \sum_{xy\in E(G_1)} \sum_{y\in V(G_2)} \Big(d_{G_1}(x) + d_{G_1}(y) + n_2 + d_{G_2}(y) + m_1\Big)^2 = n_2HZ(G_1) + m_1M_1(G_2) + (n_2 + m_1)^2 m_1 n_2 + 4m_2M_1(G_1) + 2M_1(G_1)(n_2 + m_1)n_2 + 2(n_2 + m_1)2m_2m_1$.

$I_4 = \sum_{xy\in E(G_2)} (d_{G_2}(x) + d_{G_2}(y) + 2m_1)^2 = HZ(G_2) + 4m_1^2 m_2 + 4m_1M_1(G_2)$.

$I_5 = \sum_{xy\in E(G_1)} (d_{G_2}(x) + m_1 + d_{G_2)}(y) + m_1)^2 = 4HZ(G_1)$.

Adding I_1 to I_5, we obtain the required result.

3. Conclusion

The H-invariant of edge version of new join graphs which are related to derived graphs are studied. In future, we will concentrate another graph invariants for these graph operations.

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