Y-index of some graph operations

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Abstract
Topological indices have important role in theoretical chemistry. Among the all topological indices the Zagreb indices have been used more considerably than any other topological indices in chemical literature. In this study, the Y-index for some special graphs, and graph operations has been computed, that have been applied to compute the Y-index for Nano-tube and Nano-torus. Also the strong/good correlation coefficient between the Y-index and some physical and chemical properties as Acentric factor (Acenfac), Entropy (S),Enthalpy of vaporization (HVAP) and Standard enthalpy of vaporisation (DHVAP) have been appeared.

Keywords: Zagreb indices, Hyper-Zagreb index, F-index, Y-index, graph operations.

1. INTRODUCTION

Chemical graph theory which is a fascinating branch of graph theory has many applications related to chemistry. A topological index which is a numerical quantity derived from the chemical graph of a molecule is used to modelling chemical and physical properties of molecules in QSAR/QSPR researches [4].

Throughout this paper, we consider a finite connected graph $G$ that has no loops or multiple edges. The vertex and the edge sets of a graph $G$ are denoted by $V(G)$ and $E(G)$, respectively. The degree of the vertex $\alpha$ is a number of edges joined with this vertex denoted by $\delta(\alpha)$. The distance between any two vertices $a$ and $b$ in $V(G)$ is denoted by $d(a,b)$ and it is defined as the number of edges in a shortest path, connecting the vertices $a$ and $b$.

In practical applications, Zagreb Indices are among the best applications to recognize the physical properties, and chemical reactions. First Zagreb index $M_1(G)$, and Second Zagreb index $M_2(G)$ were firstly considered by I. Gutman and N.Trinajstic in 1972 [2, 6]. They are defined as:

$$M_1(G) = \sum_{v \in V(G)} \delta_G^2(v)$$

$$= \sum_{uv \in E(G)} \delta_G(u) + \delta_G(v)$$

$$M_2(G) = \sum_{uv \in E(G)} \delta_G(u) \delta_G(v)$$

In 2005, Li and Zheng [1] introduced the first general Zagreb index as:

$$M_1^{\alpha+1}(G) = \sum_{v \in V(G)} \delta_G^{\alpha+1}(v) = \sum_{uv \in E(G)} \delta_G^\alpha(u) + \delta_G^\alpha(v)$$

In 2013, Shirdel et al [8, 9, 17], introduced distance-based of Zagreb indices named Hyper-Zagreb index as:

$$HM(G) = \sum_{uv \in E(G)} (\delta_G^2(u) + \delta_G^2(v))^2$$

Furtula and Gutman in 2015 introduced forgotten index (F-index) [13, 15] which defined as:

$$F(G) = \sum_{uv \in E(G)} (\delta_G^2(u) + \delta_G^2(v))$$

In 2018, computed exact formulas for the Zagreb and Hyper-Zagreb indices of Some Molecular Graphs by S. Ghofadi and M. Ghob耽inejad. They defined a new distance-based of Zagreb indices named Forgotton topological index or hyper F-index defined as, [14]:

$$HF(G) = \sum_{uv \in E(G)} [\delta_G^2(u) + \delta_G^2(v)]^2$$

Also in 2018, Nilanjan De use modern index to calculate the F-index and coindex Of Some Derived Graphs [12], it’s special of first general Zagreb index where $\alpha = 3$,

$$M_1^3(G) = \sum_{uv \in E(G)} \delta_G^3(u) + \delta_G^3(v).$$

But this index for some special graphs or some graph operations and it’s applications didn’t study yet. Therefore, in this paper, we named this index ‘Yemen index’ or “Y-index”. We will present some exact formulae of the Y-index for some special graphs and some graph binary operations such as tensor product $G_1 \otimes G_2$, Cartesian product $G_1 \times G_2$, composition $G_1 \circ G_2$, strong product $G_1 \ast G_2$, disjunction $G_1 \lor G_2$, symmetric difference $G_1 \oplus G_2$, of graphs. We will compare some topological indices with the Y-index by using strong $l$ good correlation coefficient acquired from the chemical graphs of octane isomers. Also we will apply some results to compute the Y-index for some classes of nano-structures such as nano-tube and nano-torus.
Definition 1.1: The Y-index of a graph $G$ define as;

$$Y(G) = \sum_{u \in V(G)} \delta_G^1(u) = \sum_{u \in E(G)} [\delta_G^1(u) + \delta_G^2(v)]$$

Lemma 1.2: Let $G_1$ and $G_2$ be graphs and $|V(G_i)| = p_i: i = 1, 2$.

Then [10, 16]

1. $\delta_{G_1 \otimes G_2}(u, v) = \delta_{G_1}(u)\delta_{G_2}(v)$
2. $\delta_{G_1 \times G_2}(u, v) = \delta_{G_1}(u) + \delta_{G_2}(v)$
3. $\delta_{G_1 \circ G_2}(u, v) = p_2\delta_{G_1}(u) + \delta_{G_2}(v)$
4. $\delta_{G_1 \ast G_2}(u, v) = \delta_{G_1}(u) + \delta_{G_2}(v) + \delta_{G_1}(u)\delta_{G_2}(v)$
5. $\delta_{G_1 \vee G_2}(u, v) = p_2\delta_{G_1}(u) + p_2\delta_{G_2}(v) - \delta_{G_1}(u)\delta_{G_2}(v)$
6. $\delta_{G_1 \oplus G_2}(u, v) = p_2\delta_{G_1}(u) + p_2\delta_{G_2}(v) - 2\delta_{G_1}(u)\delta_{G_2}(v)$

Any unexplained terminology is standard, typically as in [2, 3, 5, 7, 11].

2. BASIC PROPERTIES OF THE Y-INDEX

In this part, we give the Y-index of some special graphs as: complete graph $K_n$, cycle $C_n$, path $P_n$, complete bipartite graph $K_{m,n}$, and conical graph $C_{m,n}$ (cf. Fig. 1).

1. $Y(K_n) = n(n - 1)^4$
2. $Y(C_n) = 16n$
3. $Y(P_n) = 16n - 30$
4. $Y(K_{m,n}) = mn(m^3 + n^3)$
5. $Y(C_{m,n}) = n(n^3 + 128m - 47)$

Example 2.1: Let $G_1, G_2$ be the four and six atoms of carbon from Chemical compounds: Methylcyclopropane and Methylcyclopentane respectively depicted in Figure 2. Thus,

$$Y(G_1) = \sum_{v \in V(G_1)} \delta_{G_1}^4(v) = (1)^4 + (3)^4 + 2(2)^4 = 114,$$

$$Y(G_2) = \sum_{v \in V(G_2)} \delta_{G_2}^4(v) = (1)^4 + (3)^4 + 4(2)^4 = 146.$$
correlations, i.e., Table 3. is shown that the Y-index is octane isomers for which give reasonably highly or good correlated with the Enthalpy of vaporization (HVAP) \(|r| = 0.950848503\) and also with the entropy \(|r| = 0.944776767\) of octane isomers, and it is shown that the Y-index is good correlated with the Enthalpy of vaporization (HVAP) \(|r| = 0.851856551\) and also with the Standard enthalpy of vaporisation (DHVAP) \(|r| = 0.906174441\) of octane isomers. We can say that the Y-index is possible tools for QSPR researches.

### Table 1: Some physicochemical properties and topological indices of octane isomers

<table>
<thead>
<tr>
<th>MolID</th>
<th>AcenFac</th>
<th>S</th>
<th>HVAP</th>
<th>DHVAP</th>
<th>(M_1)</th>
<th>(M_2)</th>
<th>(F)</th>
<th>(HM)</th>
<th>(Y)</th>
<th>(HF)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CS - 01</td>
<td>0.397898</td>
<td>111.67</td>
<td>73.19</td>
<td>9.915</td>
<td>26</td>
<td>24</td>
<td>50</td>
<td>98</td>
<td>98</td>
<td>370</td>
</tr>
<tr>
<td>CS - 02</td>
<td>0.377916</td>
<td>109.84</td>
<td>70.30</td>
<td>9.484</td>
<td>28</td>
<td>26</td>
<td>62</td>
<td>114</td>
<td>148</td>
<td>586</td>
</tr>
<tr>
<td>CS - 03</td>
<td>0.371002</td>
<td>111.26</td>
<td>71.3</td>
<td>9.521</td>
<td>28</td>
<td>27</td>
<td>62</td>
<td>116</td>
<td>148</td>
<td>616</td>
</tr>
<tr>
<td>CS - 04</td>
<td>0.371504</td>
<td>109.32</td>
<td>70.91</td>
<td>9.483</td>
<td>28</td>
<td>27</td>
<td>62</td>
<td>116</td>
<td>148</td>
<td>616</td>
</tr>
<tr>
<td>CS - 05</td>
<td>0.362472</td>
<td>109.43</td>
<td>71.7</td>
<td>9.476</td>
<td>28</td>
<td>28</td>
<td>62</td>
<td>118</td>
<td>148</td>
<td>646</td>
</tr>
<tr>
<td>CS - 06</td>
<td>0.339426</td>
<td>103.42</td>
<td>67.7</td>
<td>8.915</td>
<td>32</td>
<td>30</td>
<td>92</td>
<td>152</td>
<td>308</td>
<td>1372</td>
</tr>
<tr>
<td>CS - 07</td>
<td>0.348247</td>
<td>108.02</td>
<td>70.2</td>
<td>9.272</td>
<td>30</td>
<td>30</td>
<td>74</td>
<td>134</td>
<td>198</td>
<td>882</td>
</tr>
<tr>
<td>CS - 08</td>
<td>0.344223</td>
<td>106.98</td>
<td>68.5</td>
<td>9.029</td>
<td>30</td>
<td>29</td>
<td>74</td>
<td>132</td>
<td>198</td>
<td>832</td>
</tr>
<tr>
<td>CS - 09</td>
<td>0.35683</td>
<td>105.72</td>
<td>68.6</td>
<td>9.051</td>
<td>30</td>
<td>28</td>
<td>74</td>
<td>130</td>
<td>198</td>
<td>802</td>
</tr>
<tr>
<td>CS - 10</td>
<td>0.322596</td>
<td>104.74</td>
<td>68.5</td>
<td>8.973</td>
<td>32</td>
<td>32</td>
<td>92</td>
<td>156</td>
<td>308</td>
<td>1492</td>
</tr>
<tr>
<td>CS - 11</td>
<td>0.340345</td>
<td>106.59</td>
<td>70.2</td>
<td>9.316</td>
<td>30</td>
<td>31</td>
<td>74</td>
<td>136</td>
<td>198</td>
<td>912</td>
</tr>
<tr>
<td>CS - 12</td>
<td>0.332433</td>
<td>106.06</td>
<td>69.7</td>
<td>9.209</td>
<td>30</td>
<td>31</td>
<td>74</td>
<td>136</td>
<td>198</td>
<td>912</td>
</tr>
<tr>
<td>CS - 13</td>
<td>0.306899</td>
<td>101.48</td>
<td>69.3</td>
<td>9.081</td>
<td>32</td>
<td>34</td>
<td>92</td>
<td>160</td>
<td>308</td>
<td>1564</td>
</tr>
<tr>
<td>CS - 14</td>
<td>0.300816</td>
<td>101.31</td>
<td>67.3</td>
<td>8.826</td>
<td>34</td>
<td>35</td>
<td>104</td>
<td>174</td>
<td>358</td>
<td>1786</td>
</tr>
<tr>
<td>CS - 15</td>
<td>0.30537</td>
<td>104.09</td>
<td>64.87</td>
<td>8.402</td>
<td>34</td>
<td>32</td>
<td>104</td>
<td>168</td>
<td>358</td>
<td>1636</td>
</tr>
<tr>
<td>CS - 16</td>
<td>0.293177</td>
<td>102.06</td>
<td>68.1</td>
<td>8.897</td>
<td>34</td>
<td>36</td>
<td>104</td>
<td>176</td>
<td>358</td>
<td>1828</td>
</tr>
<tr>
<td>CS - 17</td>
<td>0.317422</td>
<td>102.39</td>
<td>68.37</td>
<td>9.014</td>
<td>32</td>
<td>33</td>
<td>86</td>
<td>152</td>
<td>248</td>
<td>1037</td>
</tr>
<tr>
<td>CS - 18</td>
<td>0.255294</td>
<td>93.06</td>
<td>66.2</td>
<td>8.41</td>
<td>38</td>
<td>40</td>
<td>134</td>
<td>214</td>
<td>518</td>
<td>2758</td>
</tr>
</tbody>
</table>

In Table 2. We find that the correlation coefficient between the Y-index and some topological indices, then the correlation coefficient between the Y-index \(Y(G)\) and first Zagreb index \(M_1(G)\), F-index \(F(G)\), Hyper Zagreb index \(HM_1(G)\), and Hyper F-index \(HF(G)\) are highly correlated \((r \geq 0.95)\), and then the correlation coefficient between Y-index and the second Zagreb index \(M_2(G)\) is good correlated \((r \geq 0.90)\).

### Table 2: The correlation coefficients between Y-index and some topological indices of some physicochemical properties of octane isomers

<table>
<thead>
<tr>
<th>(r)</th>
<th>(M_1)</th>
<th>(M_2)</th>
<th>(F)</th>
<th>(HM)</th>
<th>(Y)</th>
<th>(HF)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Y - index)</td>
<td>0.98620</td>
<td>0.92469</td>
<td>0.99669</td>
<td>0.98899</td>
<td>1.00000</td>
<td>0.99353</td>
</tr>
</tbody>
</table>

In Table 3. We select those physicochemical properties of octane isomers for which give reasonably highly or good correlations, i.e., Table 3. is shown that the Y-index is highly correlated with the Acentric factor (AcenFac) \(|r| = 0.950848503\) and also with the entropy \(|r| = 0.944776767\) of octane isomers, and it is shown that the Y-index is
4. MAIN RESULTS

In the following section, we study the Y-index of some graph operations.

Theorem 4.1: Y-index of \((G_1 \otimes G_2)\) is given by:

\[ Y(G_1 \otimes G_2) = Y(G_1)Y(G_2) \]

Proof. By definition of Y-index and Lemma 1.2, we have

\[
Y(G_1 \otimes G_2) = \sum_{(u,v) \in V(G_1) \times V(G_2)} [\delta_{G_1 \otimes G_2}(u,v)]^4 = \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta_{G_1}(u)\delta_{G_2}(v)]^4
\]

\[
= \sum_{u \in V(G_1)} [\delta_{G_1}(u)]^4 \sum_{v \in V(G_2)} [1] + \sum_{u \in V(G_1)} [1] \sum_{v \in V(G_2)} [\delta_{G_2}(v)]^4 + 4 \sum_{u \in V(G_1)} [\delta_{G_1}(u)]^3 \sum_{v \in V(G_2)} \delta_{G_2}(v)
\]

\[
= p_2 Y(G_1) + n_1 Y(G_2) + 8q_1 F(G_2) + 8q_2 F(G_1) + 6M_1(G_1)M_1(G_2)
\]

Theorem 4.2: Y-index of \((G_1 \times G_2)\) is given by:

\[ Y(G_1 \times G_2) = p_2 Y(G_1) + p_1 Y(G_2) + 8q_1 F(G_2) + 8q_2 F(G_1) + 6M_1(G_1)M_1(G_2) \]

Proof. By definition of Y-index and Lemma 1.2, we have

\[
Y(G_1 \times G_2) = \sum_{(u,v) \in V(G_1 \times G_2)} [\delta_{G_1 \times G_2}(u,v)]^4 = \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta_{G_1}(u)\delta_{G_2}(v)]^4
\]

\[
= \sum_{u \in V(G_1)} [\delta_{G_1}(u)]^4 \sum_{v \in V(G_2)} [1] + \sum_{u \in V(G_1)} [1] \sum_{v \in V(G_2)} [\delta_{G_2}(v)]^4 + 4 \sum_{u \in V(G_1)} [\delta_{G_1}(u)]^3 \sum_{v \in V(G_2)} \delta_{G_2}(v)
\]

\[
= p_2 Y(G_1) + p_1 Y(G_2) + 8q_1 F(G_2) + 8q_2 F(G_1) + 6M_1(G_1)M_1(G_2)
\]

Theorem 4.3: Y-index of \((G_1 \circ G_2)\) is given by:

\[ Y(G_1 \circ G_2) = p_2^2 Y(G_1) + p_1 Y(G_2) + 8p_2 q_2 F(G_1) + 8p_2 q_1 F(G_2) + 6p_2^2 M_1(G_1)M_1(G_2) \]

Proof. By definition of Y-index and Lemma 1.2, we have

\[
Y(G_1 \circ G_2) = \sum_{(u,v) \in V(G_1 \circ G_2)} [\delta_{G_1 \circ G_2}(u,v)]^4 = \sum_{u \in V(G_1 \circ G_2)} [\delta_{G_1}(u)\delta_{G_2}(v)]^4
\]

\[
= \sum_{(u,v) \in V(G_1 \circ G_2)} [p_2^4 \delta_{G_1}(u) + \delta_{G_2}(v) + 6p_2^2 \delta_{G_1}(u)\delta_{G_2}(v) + 4p_2^3 \delta_{G_1}(u)\delta_{G_2}(v) + 4p_2 \delta_{G_1}(u)\delta_{G_2}(v)]
\]

\[
= p_2^5 Y(G_1) + p_1 Y(G_2) + 8p_2 q_2 F(G_1) + 8p_2 q_1 F(G_2) + 6p_2^2 M_1(G_1)M_1(G_2)
\]

Theorem 4.4: Y-index of \((G_1 \ast G_2)\) is given by:

\[ Y(G_1 \ast G_2) = Y(G_1)[4F(G_2) + 6M_1(G_2) + 8q_2 + p_2] + 4F(G_1)[3M_1(G_2) + 2q_2]
\]

\[ + Y(G_2)[4F(G_1) + 6M_1(G_1) + 8q_1 + p_1] + 4F(G_2)[3M_1(G_1) + 2q_1]
\]

\[ + Y(G_1)Y(G_2) + 12F(G_1)F(G_2) + 6M_1(G_1)M_1(G_2).
\]
Proof. By definition of Y-index and Lemma 1.2, we have

\[
Y(G_1 \star G_2) = \sum_{(u,v) \in V(G_1 \star G_2)} [\delta(G_1 + G_2)(u,v)]^4 = \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta(G_1)(u) + \delta(G_2)(v) + \delta(G_1)(u) \delta(G_2)(v)]^4
\]

\[
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [\delta(G_1)(u) + \delta(G_2)(v) + 6\delta(G_1)(u) \delta(G_2)(v) + 12\delta(G_1)(u) \delta(G_2)(v)]^4
\]

\[
= p_2 Y(G_1) + p_1 Y(G_2) + 4Y(G_1)(2q_2) + 4Y(G_1)(2q_1) + 4Y(G_2)(2q_2) + 4Y(G_2)(2q_1)
\]

\[
= p_2 Y(G_1) + p_1 Y(G_2) + 12p_1p_2F(G_1)F(G_2) + 6p_1p_2M_1(G_1)M_1(G_2).
\]

Theorem 4.5: Y-index of \((G_1 \cup G_2)\) is given by:

\[
Y(G_1 \cup G_2) = p_1 Y(G_2) [p_1^4 + 6p_1 M_1(G_1) - 8p_1^2q_1 - 4F(G_1)] + 4p_1^2p_2 F(G_2)[2p_1 q_1 - 3M_1(G_1)]
\]

\[
+ p_2 Y(G_1) [p_2^4 + 6p_2 M_1(G_2) - 8p_2^2q_2 - 4F(G_2)] + 4p_2^2p_1 F(G_1)[2p_2 q_2 - 3M_1(G_2)]
\]

\[
+ Y(G_1) Y(G_2) + 12p_1p_2 F(G_1) F(G_2) + 6p_1p_2 M_1(G_1) M_1(G_2).
\]

Proof. By definition of Y-index and Lemma 1.2, we have

\[
Y(G_1 \cup G_2) = \sum_{(u,v) \in V(G_1 \cup G_2)} [\delta(G_1 \cup G_2)(u,v)]^4 = \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [p_2 \delta(G_1)(u) + p_1 \delta(G_2)(v) - \delta(G_1)(u) \delta(G_2)(v)]^4
\]

\[
= \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} [p_1^4 \delta(G_1)(u) + p_2^4 \delta(G_2)(v) + 6p_1^2p_2^2 \delta(G_1)(u) \delta(G_2)(v) + 12p_1p_2 \delta(G_1)(u) \delta(G_2)(v)]^4
\]

\[
= p_1 Y(G_2) [p_1^4 + 6p_1 M_1(G_1) - 8p_1^2q_1 - 4F(G_1)] + 4p_1^2p_2 F(G_2)[2p_1 q_1 - 3M_1(G_1)]
\]

\[
+ p_2 Y(G_1) [p_2^4 + 6p_2 M_1(G_2) - 8p_2^2q_2 - 4F(G_2)] + 4p_2^2p_1 F(G_1)[2p_2 q_2 - 3M_1(G_2)]
\]

\[
+ Y(G_1) Y(G_2) + 12p_1p_2 F(G_1) F(G_2) + 6p_1p_2 M_1(G_1) M_1(G_2).
\]

Theorem 4.6: Y-index of \((G_1 \odot G_2)\) is given by:

\[
Y(G_1 \odot G_2) = p_1 Y(G_2) [p_1^4 + 24p_1 M_1(G_1) - 16p_1^2q_1 - 32F(G_1)] + 8p_1^2p_2 F(G_2)[2p_1 q_1 - 3M_1(G_1)]
\]

\[
+ p_2 Y(G_1) [p_2^4 + 24p_2 M_1(G_2) - 16p_2^2q_2 - 32F(G_2)] + 8p_2^2p_1 F(G_1)[2p_2 q_2 - 3M_1(G_2)]
\]

\[
+ 16Y(G_1) Y(G_2) + 48p_1p_2 F(G_1) F(G_2) + 6p_1p_2 M_1(G_1) M_1(G_2).
\]

Proof. By using a similar method, one can prove the exact formula for the Y-index of symmetric difference of graphs.
Example 4.7: Khalifeh, M. H., et al. [18] computed the Y-index of C4 nanotubes and nanotori. In this example, we compute these molecular graphs. Suppose R and S denote a C4 nanotube and nanotorus, respectively. Then $R = P_n \times C_m$ and $S = C_n \times C_m$, by Theorem 4.2:

$$Y(R) = Y(P_n \times C_m) = 224nm + 16n - 304m - 30$$

where

$$G_1 \equiv P_n, \quad p_1 = n, q_1 = n - 1, M_1(P_n) = 4n - 6, F(P_n) = 8n - 14, Y(P_n) = 16n - 30,$$

$$G_1 \equiv C_m, \quad p_2 = q_2 = m, M_1(C_m) = 4m, F(C_m) = 8m, Y(C_m) = 16m$$

Similar we have

$$Y(S) = Y(C_n \times C_m) = 192nm + 16n + 16m$$

Example 4.8: Let $P_2, P_3$ denote a paths with 2 and 3 vertices, respectively. By theorem 4.1-6. we have The Y-index of some graph operations of $P_2, P_3$ in table 4.

<table>
<thead>
<tr>
<th>$G$</th>
<th>$P_2 \odot P_3$</th>
<th>$P_2 \times P_3$</th>
<th>$P_2 \odot P_3$</th>
<th>$P_2 \star P_3$</th>
<th>$P_2 \oplus P_3$</th>
<th>$P_2 \lor P_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y(G)$</td>
<td>96</td>
<td>226</td>
<td>2274</td>
<td>1574</td>
<td>486</td>
<td>2274</td>
</tr>
</tbody>
</table>

5. CONCLUDING REMARKS

In this paper, a new index was introduced from the Zagreb index family, named that Y-index. it has investigated the basic mathematical properties of the Y-index and obtained explicit formula for their values under several graph operations. The strong correlation coefficient between Y-index and some physico-chemical properties as Acentric factor has been Appeared. Here we mention some possible directions for future research as multiplicative Y-index.

REFERENCES


