WIENER, HYPER-WIENER, TRATCH-STANKEVICH-ZEFIROV INDEX FOR CARTESIAN PRODUCT OF GRAPHS

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ABSTRACT:

A topological index is the graph invariant numerical descriptor calculated from a molecular graph representing a molecule. Classical Zagreb and Wiener indices and the recently introduced Zagreb coindices are topological indices related to the atom – atom connectivity of the molecular structure represented by the graph *G*. We explore here their basic mathematical properties and present explicit formulae for these new graph invariants under several graph operations.

KEYWORDS:

NANOTUBES, NANOTORUS OR NANOTORI, TSZ OF C_4 NANTOUBES AND NANOTORUS OR NANOTORI.

INTRODUCTION:

Graph theory is a branch of mathematics started by Euler as early as 1736. It took a hundred years before the second important contribution of Kirchhoff had been made for the analysis of electrical networks. Cayley and Sylvester discovered several properties of special types of graphs known as trees. Poincare defined in principle what is known nowadays as the incidence matrix of a graph.

DEFINITION

Definition 1

The Cartesian product G×H of graphs G and H is a graph such that V(G×H)=V(G)×V(H) and any two vertices (a,b) and (u,v) are adjacent in G×H if and only if either a=u and b is adjacent with v, or b=v and a is adjacent with u.

Definition 2

For a product G×H, the projection $p_G : G \times H \rightarrow G$ is defined by $p_G: (g, h) \rightarrow g$, $g \in G$ and $h \in H$. It is clear what we mean by p_H. Under the projections p_G or p_H, the image of an edge is an edge or a single vertex. Such mappings are weak homomorphisms (Wilfried 1941).

Definition 3

For a path P of G×H consisting of a single edge e, we clearly have

$$|E(P)| = |E(p_G P)| + |E(p_H P)|$$

because either $p_G P$ or $p_H P$ consists of a single vertex. If P is not a single edge, it may happen that two edges e and f of P have the same projection into one of the factors. Thus,

$$|E(P)| \geq |E(p_G P)| + |E(p_H P)|$$

SOME THEOREMS BASED ON WIENER TYPE INVARIANTS

Lemma :1

G×H is connected if and only if G and H are connected.

Proof

Suppose G×H is connected. We have to prove that both G and H are connected. Clearly, it suffices to prove it for G.

Let a and b be any two vertices of G, and let cϵH be arbitrary. Then there is a path P in G×H from (a,c) to (b,c), and $p_G P \subseteq G$ contains a path from a to b.

Conversely, assume that G and H are connected. We have to show that there is a path between any two arbitrarily chosen vertices (a,c) and (b,d) of G×H. Let R be a a,b-path and S be c,d-path. Then,

$(R\times\{c\})\cup(\{b\}\times S)$ is a $(a,c),(b,d)$ is a path.

Hence G×H is connected.

Lemma :2

Let G and H be graphs. If ((a,c).(b,d)) $\in$ V(G×H) then we have, $d_{G\times H}((a,c),(b,d))=d_G(a,b)+d_H(c,d)$.

Proof

We know that, $d_G(a,b)$ is the distance between two vertices a and b of a graph G and $d_H(c,d)$is the distance between two vertices c and d of a graph H. i.e. $d_G(a,b)$ is the number of edges on a shortest a,b-path and $d_H(c,d)$ is the number of edges on a shortest c,d-path.

Let P be a shortest ((a,c),(b,d)) path in G×H. By Definition 5.1.4,

$$d_{G\times H}((a,c),(b,d))\geq d_G(a,b)+d_H(c,d) \qquad (5.1)$$

Furthermore, if R is a shortest a,b-path in G and S is a shortest c,d-path in H. Then $(R\times\{c\})\cup(\{b\}\times S)$ is a $(a,c),(b,d)$ – path of length $d_G(a,b)+d_H(c,d)$.

Hence, $$d_{G\times H}((a,c),(b,d))\leq d_G(a,b)+d_H(c,d) \qquad (5.2)$$

From (5.1) and (5.2) we get,

$$d_{G\times H}((a,c),(b,d))=d_G(a,b)+d_H(c,d).$$

Lemma :3

Suppose G and H are connected graphs, $|V(G)| = m$, $|V(H)| = n$ and λ is a positive integer. Then

$$W_\lambda(G\times H)=m^2W_\lambda(H)+2\binom{\lambda}{1}W(G)W_{\lambda-1}(H)+2\binom{\lambda}{2}W_2(G)W_{\lambda-2}(H)$$
$$+......+2\binom{\lambda}{\lambda-1}W_{\lambda-1}(G)W(H)+n^2W_\lambda(G).$$

Proof

Suppose $(u_1,u_2,\dots,u_m)$ and $(v_1,v_2,\dots,v_n)$ are vertices of G and H respectively. Given G and H are connected graphs. By definition of W_λ,

$$W_\lambda(G\times H)=\sum_{\{u,v\}} d^\lambda_{G\times H}(u,v)$$

$$W_\lambda(G\times H)=\frac{1}{2}\sum_{(u_i,v_k)}\sum_{(u_j,v_l)} d^\lambda_{G\times H}\big((u_i,v_k),(u_j,v_l)\big)$$

$$=\frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}\big(d_G(u_i,u_j)+d_H(v_k,v_l)\big)^\lambda$$

$$=\frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}\left[\sum_{r=0}^{\lambda}\binom{\lambda}{r} d^r_G(u_i,u_j)d^{\lambda-r}_H(v_k,v_l)\right]$$

$$=\frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}\left[\begin{array}{l}\binom{\lambda}{0} d^0_G(u_i,u_j)d^{\lambda-0}_H(v_k,v_l)+\binom{\lambda}{1} d^1_G(u_i,u_j)d^{\lambda-1}_H(v_k,v_l)+\\ \binom{\lambda}{2} d^2_G(u_i,u_j)d^{\lambda-2}_H(v_k,v_l)+.....+\binom{\lambda}{\lambda-1} d^{\lambda-1}_G(u_i,u_j)d^1_H(v_k,v_l)\\ \qquad\qquad +d^\lambda_G(u_i,u_j)\end{array}\right]$$

$$=\frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}d^\lambda_H(v_k,v_l)+\frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}\binom{\lambda}{1}d_G(u_i,u_j)d^{\lambda-1}_H(v_k,v_l)$$
$$+\frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}\binom{\lambda}{2}d^2_G(u_i,u_j)d^{\lambda-2}_H(v_k,v_l)+..........$$
$$+\frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}\binom{\lambda}{\lambda-1}d^{\lambda-1}_G(u_i,u_j)d_H(v_k,v_l)+\frac{1}{2}\sum_{k,l=1}^{n}\sum_{i,j=1}^{m}d^\lambda_G(u_i,u_j)$$

$$=\sum_{i,j=1}^{m}W_\lambda(H)+2\binom{\lambda}{1}W(G)W_{\lambda-1}(H)+2\binom{\lambda}{2}W_2(G)W_{\lambda-2}(H)$$
$$+......+2\binom{\lambda}{\lambda-1}W_{\lambda-1}(G)W(H)+\sum_{k,l=1}^{n}W_\lambda(G)$$

$$W_\lambda(G\times H)=m^2W_\lambda(H)+2\binom{\lambda}{1}W(G)W_{\lambda-1}(H)+2\binom{\lambda}{2}W_2(G)W_{\lambda-2}(H)$$
$$+......+2\binom{\lambda}{\lambda-1}W_{\lambda-1}(G)W(H)+n^2W_\lambda(G).$$

NANOTUBES

Carbon nanotubes are hollow, cylindrical nanostructures composed of single sheet of carbon atoms. Carbon nanotubes have exceptional electrical, physical and thermal properties. Carbon nanotubes are stronger than steel and 200 times lighter than steel. Carbon nanotubes are 10,000 times thinner than human hair.

Example:1

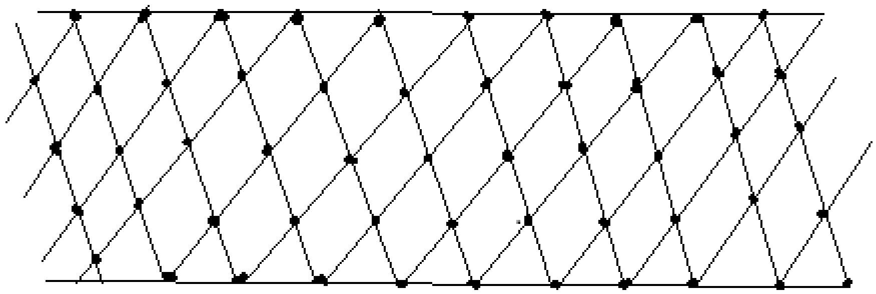


Figure 5.3 C_4 Nanotubes

NANOTORUS OR NANOTORI

Nanotorous is theoretically describes as carbon nanotube bent into a torus (doughnut shape). Nanotorus are predicted to have many unique properties such as magnetic moments, thermal stability etc. vary widely depending on radius of the torus and the radius of the tube.

Example :1

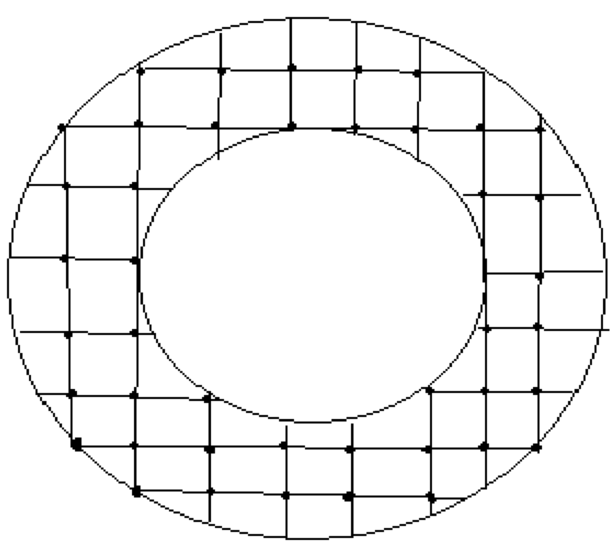


Figure 5.3 C_4 Nanotorus or Nanotori

5.5 TSZ OF C_4 NANTOUBES AND NANOTORUS OR NANOTORI

Corollary :1

The Tratch-Stankevich-Zefirov index of C_4 nanotubes and nanotori are computed as follows:

(i) If m is even then,

$$TSZ(P_n \times C_m) = \frac{1}{120}m^2n^5 + \frac{1}{24}m^2n^4 + \frac{1}{18}m^2n^3 - \frac{23}{360}m^2n + \frac{1}{384}m^5n^2 + \frac{1}{24}m^3n^2$$
$$+\frac{1}{144}m^4n^3 + \frac{1}{48}m^4n^2 - \frac{1}{144}m^4n + \frac{1}{96}m^3n^4 + \frac{1}{24}m^3n^3 - \frac{1}{24}m^3n.$$

Proof

Using corollary (5.2.4),

$$TSZ(P_n \times C_m) = |V(C_m)|^2 TSZ(P_n) + |V(P_n)|^2 TSZ(C_m) + W(P_n)W_2(C_m)$$
$$+W_2(P_n)W(C_m) + 2W(P_n)W(C_m)$$

$$TSZ(P_n \times C_m) = m^2TSZ(P_n) + n^2TSZ(C_m) + W(P_n)W_2(C_m)$$
$$+W_2(P_n)W(C_m) + 2W(P_n)W(C_m) \qquad (5.4)$$

If m is even then the wiener type invariant of cycle graph C_m is,

$$W_\lambda(C_m) = m\sum_{i=1}^{\frac{m}{2}-1} i^\lambda + \left(\frac{m}{2}\right)^\lambda \frac{m}{2}$$

$$W_1(C_m) = m\sum_{i=1}^{\frac{m}{2}-1} i + \left(\frac{m}{2}\right) \frac{m}{2}$$

$$= m\left[1+2+3+.....+\left(\frac{m}{2}-1\right)\right] + \frac{m^2}{4}$$

$$= \frac{m\left(\frac{m}{2}-1\right)\left(\frac{m}{2}-1+1\right)}{2} + \frac{m^2}{4}$$

$$W_1(C_m) = \frac{m^3}{8}$$

$$W_2(C_m) = m\sum_{i=1}^{\frac{m}{2}-1} i^2 + \left(\frac{m}{2}\right)^2 \frac{m}{2}$$

$$= m\left[1^2+2^2+3^2+.....+\left(\frac{m}{2}-1\right)^2\right] + \frac{m^3}{8}$$

$$=\frac{m\left(\frac{m}{2}-1\right)\left(\frac{m}{2}-1+1\right)\left[2\left(\frac{m}{2}-1\right)+1\right]}{6}+\frac{m^3}{8}$$

$$W_2(C_m)=\frac{m^4+2m^2}{24}$$

$$W_3(C_m)=m\sum_{i=1}^{\frac{m}{2}-1} i^3+\left(\frac{m}{2}\right)^3\frac{m}{2}$$

$$=m\left[1^3+2^3+3^3+.....+\left(\frac{m}{2}-1\right)^3\right]+\frac{m^4}{16}$$

$$=m\left[\frac{\left(\frac{m}{2}-1\right)\left(\frac{m}{2}-1+1\right)}{2}\right]^2+\frac{m^4}{16}$$

$$W_3(C_m)=\frac{m^5+4m^3}{64}$$

$$TSZ(C_m)=\frac{1}{6}\left[\frac{m^5+4m^3}{64}\right]+\frac{1}{2}\left[\frac{m^4+2m^2}{24}\right]+\frac{1}{3}\left[\frac{m^3}{8}\right]$$

$$TSZ(C_m)=\frac{m^5}{384}+\frac{m^4}{48}+\frac{5m^3}{96}+\frac{m^2}{24}$$

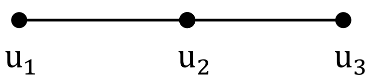
Then substituting the equation in (5.4),

$$TSZ(P_n\times C_m)=m^2\left[\frac{n^5+5n^4+5n^3-5n^2-6n}{120}\right]+n^2\left[\frac{m^5}{384}+\frac{m^4}{48}+\frac{5m^3}{96}+\frac{m^2}{24}\right]$$
$$+\left(\frac{n^3-n}{6}\right)\left(\frac{m^4+2m^2}{24}\right)+\left(\frac{n^4-n^2}{12}\right)\left(\frac{m^3}{8}\right)+2\left(\frac{m^3}{8}\right)\left(\frac{n^3-n}{6}\right)$$

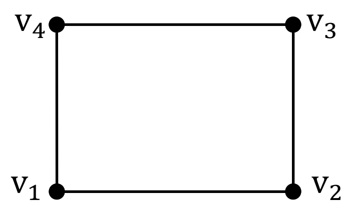
$$TSZ(P_n\times C_m)=\frac{1}{120}m^2n^5+\frac{1}{24}m^2n^4+\frac{1}{18}m^2n^3-\frac{23}{360}m^2n+\frac{1}{384}m^5n^2+\frac{1}{24}m^3n^2$$
$$+\frac{1}{144}m^4n^3+\frac{1}{48}m^4n^2-\frac{1}{144}m^4n+\frac{1}{96}m^3n^4+\frac{1}{24}m^3n^3-\frac{1}{24}m^3n.$$

Example :2

P_3:



C_4:



$P_3 \times C_4$:

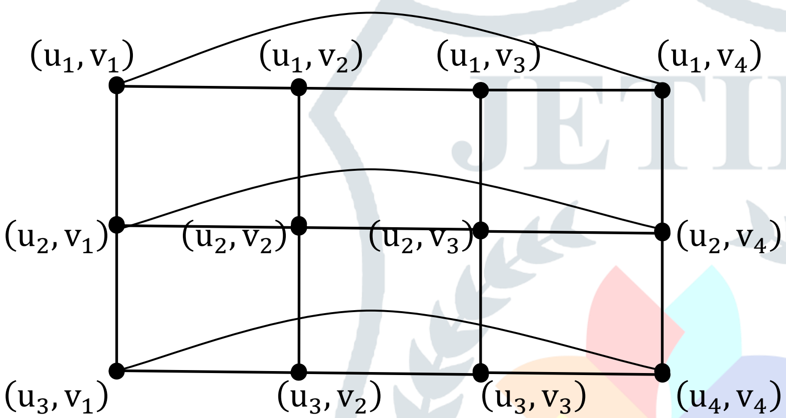


Figure 5.5 Cartesian product of P_3 and C_4

$$TSZ(P_3 \times C_4) = \frac{1084}{3}$$

(ii) If m is odd then,

$$TSZ\left(P_n \times C_m\right) = \frac{1}{120}m^2n^5 + \frac{1}{24}m^2n^4 + \frac{5}{144}m^2n^3 - \frac{1}{16}m^2n^2 - \frac{31}{720}m^2n + \frac{1}{384}m^5n^2$$

$$- \frac{11}{384}mn^2 + \frac{1}{48}m^4n^2 + \frac{5}{192}m^3n^2 + \frac{1}{144}m^4n^3 - \frac{1}{144}m^4n + \frac{1}{96}m^3n^4$$

$$- \frac{1}{96}mn^4 + \frac{1}{24}m^3n^3 - \frac{1}{24}mn^3 - \frac{1}{24}m^3n + \frac{1}{24}mn.$$

Proof

Using corollary (5.2.4),

$$TSZ(P_n \times C_m) = |V(C_m)|^2 TSZ(P_n) + |V(P_n)|^2 TSZ(C_m) + W(P_n)W_2(C_m) + W_2(P_n)W(C_m) + 2W(P_n)W(C_m)$$

$$TSZ(P_n \times C_m) = m^2 TSZ(P_n) + n^2 TSZ(C_m) + W(P_n)W_2(C_m) + W_2(P_n)W(C_m) + 2W(P_n)W(C_m) \qquad (5.5)$$

If m is odd then the wiener type invariant of cycle graph C_m is,

$$W_\lambda(C_m) = m\sum_{i=1}^{\frac{m-1}{2}} i^\lambda$$

$$W_1(C_m) = m\sum_{i=1}^{\frac{m-1}{2}} i$$

$$= m\left[1+2+\ldots+\left(\frac{m-1}{2}\right)\right]$$

$$= m\left[\frac{\left(\frac{m-1}{2}\right)\left(\frac{m-1}{2}+1\right)}{2}\right]$$

$$W_1(C_m) = \frac{m(m^2-1)}{8}$$

$$W_2(C_m) = m\sum_{i=1}^{\frac{m-1}{2}} i^2$$

$$= m\left[1^2+2^2+\ldots+\left(\frac{m-1}{2}\right)^2\right]$$

$$= m\left[\frac{\left(\frac{m-1}{2}\right)\left(\frac{m-1}{2}+1\right)\left(2\left(\frac{m-1}{2}\right)+1\right)}{6}\right]$$

$$W_2(C_m) = \frac{m^2(m^2-1)}{24}$$

$$W_3(C_m) = m\sum_{i=1}^{\frac{m-1}{2}} i^3$$

$$=m\left[1^3+2^3+\ldots+\left(\frac{m-1}{2}\right)^3\right]$$

$$=m\left[\frac{\left(\frac{m-1}{2}\right)\left(\frac{m-1}{2}+1\right)}{2}\right]^2$$

$$W_3\left(C_m\right)=\frac{m^5-2m^3+m}{64}$$

$$TSZ\left(C_m\right)=\frac{1}{6}\left[\frac{m^5-2m^3+m}{64}\right]+\frac{1}{2}\left[\frac{m^2\left(m^2-1\right)}{24}\right]+\frac{1}{3}\left[\frac{m\left(m^2-1\right)}{8}\right]$$

$$TSZ\left(C_m\right)=\frac{m^5}{384}+\frac{m^4}{48}+\frac{7m^3}{192}-\frac{m^2}{48}-\frac{15m}{384}$$

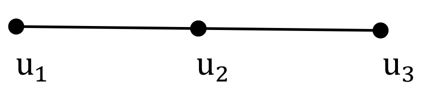
Then substituting the equation in (5.5),

$$TSZ\left(P_n\times C_m\right)=m^2\left[\frac{n^5}{120}+\frac{5n^4}{120}+\frac{5n^3}{120}-\frac{5n^2}{120}-\frac{6n}{120}\right]+n^2\left[\frac{m^5}{384}+\frac{m^4}{48}+\frac{7m^3}{192}-\frac{m^2}{48}-\frac{15m}{384}\right]$$
$$+\left[\frac{n^3-n}{6}\right]\left[\frac{m^2\left(m^2-1\right)}{24}\right]+\left[\frac{m\left(m^2-1\right)}{8}\right]\left[\frac{n^4-n^2}{12}\right]+2\left[\frac{n^3-n}{6}\right]\left[\frac{m\left(m^2-1\right)}{8}\right]$$

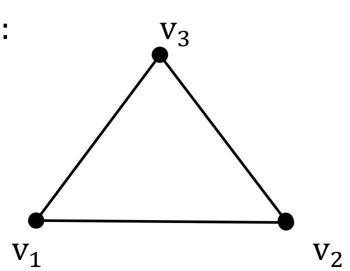
$$TSZ\left(P_n\times C_m\right)=\frac{1}{120}m^2n^5+\frac{1}{24}m^2n^4+\frac{5}{144}m^2n^3-\frac{1}{16}m^2n^2-\frac{31}{720}m^2n+\frac{1}{384}m^5n^2$$
$$-\frac{11}{384}mn^2+\frac{1}{48}m^4n^2+\frac{5}{192}m^3n^2+\frac{1}{144}m^4n^3-\frac{1}{144}m^4n+\frac{1}{96}m^3n^4$$
$$-\frac{1}{96}mn^4+\frac{1}{24}m^3n^3-\frac{1}{24}mn^3-\frac{1}{24}m^3n+\frac{1}{24}mn.$$

Example :3

P_3 :



C_3:



$P_3 \times C_3$:

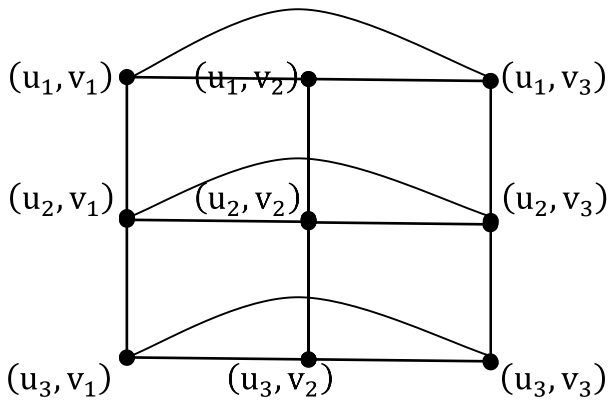


Figure 5.6 Cartesian product of P_3 and C_3

$$TSZ(P_3 \times C_3) = \frac{2161}{16}$$

(iii) If m and n are even then,

$$TSZ(C_n \times C_m) = \frac{1}{384}m^2n^5 + \frac{1}{16}m^2n^3 + \frac{1}{48}m^2n^4 + \frac{1}{12}m^2n^2 + \frac{1}{384}m^5n^2 + \frac{1}{16}m^3n^2 + \frac{1}{48}m^4n^2 + \frac{1}{192}m^4n^3 + \frac{1}{192}m^3n^4 + \frac{1}{32}m^3n^3.$$

Proof

$$TSZ(C_n \times C_m) = |V(C_m)|^2 TSZ(C_n) + |V(C_n)|^2 TSZ(C_m) + W(C_n)W_2(C_m) + W(C_m)W_2(C_n) + 2W(C_m)W(C_n)$$

$$TSZ(C_n \times C_m) = m^2 TSZ(C_n) + n^2 TSZ(C_m) + W(C_n)W_2(C_m) + W(C_m)W_2(C_n) + 2W(C_m)W(C_n) \quad (5.6)$$

Given m and are even,

$$W_1(C_m) = \frac{m^3}{8}$$

$$W_2(C_m) = \frac{m^4 + 2m^2}{24}$$

$$TSZ(C_m) = \frac{m^5}{384} + \frac{m^4}{48} + \frac{5m^3}{96} + \frac{m^2}{24}$$

Then substituting the equation in (5.6),

$$TSZ(C_n \times C_m) = m^2\left[\frac{n^5}{384}+\frac{n^4}{48}+\frac{5n^3}{96}+\frac{n^2}{24}\right]+n^2\left[\frac{m^5}{384}+\frac{m^4}{48}+\frac{5m^3}{96}+\frac{m^2}{24}\right]$$
$$+\left[\frac{n^3}{8}\right]\left[\frac{m^4+2m^2}{24}\right]+\left[\frac{m^3}{8}\right]\left[\frac{n^4+2n^2}{24}\right]+2\left[\frac{n^3}{8}\right]\left[\frac{m^3}{8}\right]$$

$$TSZ(C_n \times C_m) = \frac{1}{384}m^2n^5+\frac{1}{16}m^2n^3+\frac{1}{48}m^2n^4+\frac{1}{12}m^2n^2+\frac{1}{384}m^5n^2$$
$$+\frac{1}{16}m^3n^2+\frac{1}{48}m^4n^2+\frac{1}{192}m^4n^3+\frac{1}{192}m^3n^4+\frac{1}{32}m^3n^3.$$

CONCLUSION

In this dissertation, Basic concepts of graph theory and Introduction to chemical graph theory have been discussed. Also Zagreb indices and Wiener coindices have been explained and we have investigated their basic mathematical properties and obtained explicit formulae for computing their values under several graph operations namely Cartesian product, Disjunction, Composition, Tensor product and Normal product of graphs. Also studied the application of Tratch Stankevich Zefirov index of C_4 nanotubes and nanotorus.

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