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# MOLECULAR DESCRIPTORS OF SOME TYPES OF CHEMICAL GRAPHS

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ABSTRACT. In this section, we study the certain molecular descriptors for of Titanaia nanotubes ($TiO_2[m,n]$) and Armchair Polyhex nanotubes ($TUAC_6[m,n]$).

## 1. INTRODUCTION

Chemical graph theory is the topological branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena. Studying topological properties of fullerenes, nanotubes, nanocones, nanostars etc. are emerging topics in nanotechnology, theoretical chemistry and mathematical chemistry. Degree-based molecular descriptors provide a better correlation for certain physico-chemical properties of chemical compounds.For more details about this see [2–8].

A chemical graph is a simple graph in which the vertices correspond to the atoms and the edges correspond to the bonds between them in a chemical compound. The degreed $(u)$ of a vertex $u$ in a graph $G$ is the number of vertices adjacent to $u$ in $G$.

The following invariants are defined and studied by various researchers.

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(1) First and second Zagreb invariants:

$$M_1(G) = \sum_{u\in V(G)} (d_G(u))^2 = \sum_{u,v\in E(G)} (d_G(u) + d_G(v))$$

and

$$M_2(G) = \sum_{u,v\in E(G)} d_G(u)d_G(v).$$

(2) Geometric-arithmetic invariant:

$$GA(G) = \sum_{i=1}^{|E(G)|} \sigma_i \text{ where } \sigma_i = \sum_{u,v\in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)}.$$

(3) Atom- bond connectivity invariant:

$$ABC(G) = \sum_{i=1}^{|E(G)|} \beta_i \text{ where } \beta_i = \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}}.$$

(4) Augmented Zagreb invariant:

$$AZI(G) = \sum_{i=1}^{|E(G)|} \theta_i \text{ where } \theta_i = \sum_{u,v\in E(G)} \left(\frac{d_G(u)d_G(v)}{d_G(u) + d_G(v) - 2}\right)^3.$$

(5) Fifth geometric-arithmetic invariant:

$$GA_5(G) = \sum_{i=1}^{|E(G)|} \sigma_i^{'} \text{ where } \sigma_i^{'} = \sum_{u,v\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u + S_v - 2}.$$

(6) Fourth member of the class of $ABC$ invariant:

$$ABC_4(G) = \sum_{i=1}^{|E(G)|} \beta_i^{'} \text{ where } \beta_i^{'} = \sum_{u,v\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_uS_v}}.$$

(7) Sanskruti invariant $S(G)$:

$$S(G) = \sum_{i=1}^{|E(G)|} \theta_i^{'} \text{ where } \theta_i^{'} = \sum_{u,v\in E(G)} \left(\frac{S_uS_v}{S_u + S_v - 2}\right)^3.$$

## 2. TITANAIA NANOTUBES $TiO_2[m,n]$

Titania is comprehensively discussed in materials science. Titania nanotubes were systematically synthesized during the last 1015 years using different methods and carefully studied as prospective technological materials. Since the growth mechanism for $TiO_2$ nanotubes is still not well defined, their comprehensive theoretical studies attract enhanced attention. $TiO_2$ sheets with a thickness of a few atomic layers were found to be remarkably stable [1], see Figure 1. From the structure of the molecular graph $TiO_2[m,n]$, we have the number

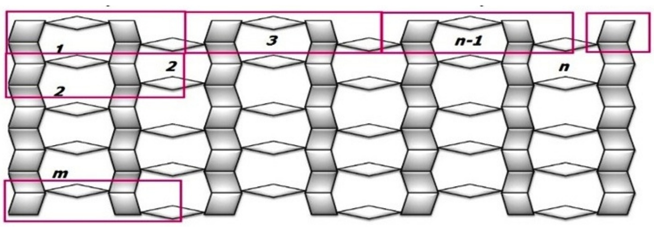


FIGURE 1. Titanaia nanotubes $TiO_2[m,n]$

of vertices are $6n(m+1)$. The following table gives details for types of edges, their numbers and the value of $\sigma_i, \beta_i, \theta_i$ of a molecular graph $TiO_2[m,n]$.

TABLE 1. $G = TiO_2$ nanotubes

| Number of edges | $\sigma_i$ | $\beta_i$ | $\theta_i$ | Types of edges |
|---|---|---|---|---|
| 6n | $\frac{2\sqrt{2}}{3}$ | $\sqrt{\frac{1}{2}}$ | 8 | (2,4) |
| 4mn+4n | $\frac{2\sqrt{10}}{7}+\frac{2\sqrt{12}}{7}$ | $\sqrt{\frac{1}{2}}+\sqrt{\frac{5}{12}}$ | 21.824 | (2,5) and (3,4) |
| 6mn-2n | $\frac{\sqrt{15}}{4}$ | $\sqrt{\frac{2}{5}}$ | 15.625 | (3,5) |

From the definitions of $GA$ invariant, $ABC$ invariant, $AZI$ invariant and the Table 1, we obtain the following result.

**Theorem 2.1.** *Let $G = TiO_2$ nanotubes. Then*

(i) $GA(G) = 2n\left(5\sqrt{0.5}+\sqrt{\frac{5}{3}}-\sqrt{0.4}\right)+2mn\left(2\sqrt{0.5}+\sqrt{\frac{5}{3}}+3\sqrt{0.4}\right).$

(ii) $ABC(G) = 2n\left(\frac{22}{7}\sqrt{2}+\frac{5}{7}\sqrt{10}-\frac{\sqrt{15}}{4}\right)+2mn\left(\frac{4}{7}\sqrt{10}+\frac{8}{7}\sqrt{2}+\frac{3}{4}\sqrt{15}\right).$

(iii) $AZI(G) = (62.574)n + (181.046)mn.$

TABLE 2. Let $G = TiO_2[m,n]$ nanotubes.

| Number of edges | $\sigma_i^{'}$ | $\beta_i^{'}$ | $\theta_i^{'}$ | Types of edges |
|---|---|---|---|---|
| 2 | $\frac{2\sqrt{50}}{15}$ | $\sqrt{\frac{13}{50}}$ | $\left(\frac{50}{13}\right)^3$ | (10,5) |
| 2 | $\frac{\sqrt{35}}{6}$ | $\sqrt{\frac{14}{63}}$ | $\left(\frac{7}{2}\right)^3$ | (7,5) |
| 2n | $\frac{3\sqrt{7}}{8}$ | $\sqrt{\frac{17}{90}}$ | $\left(\frac{63}{14}\right)^3$ | (7,9) |
| 4n | $\frac{12\sqrt{2}}{17}$ | $\sqrt{\frac{20}{117}}$ | $\left(\frac{72}{15}\right)^3$ | (8,9) |
| 2n | $\frac{6\sqrt{10}}{19}$ | $\sqrt{\frac{21}{130}}$ | $\left(\frac{90}{17}\right)^3$ | (10,9) |
| 6m | $\frac{\sqrt{99}}{10}$ | $\sqrt{\frac{2}{7}}$ | $\left(\frac{117}{20}\right)^3$ | (11,9) |
| 3m | $\frac{\sqrt{117}}{11}$ | $\sqrt{\frac{15}{72}}$ | $\left(\frac{117}{20}\right)^3$ | (13,9) |
| 2n | $\frac{\sqrt{91}}{10}$ | $\sqrt{\frac{18}{99}}$ | $\left(\frac{91}{18}\right)^3$ | (7,13) |
| 4mn+2n | $\frac{2\sqrt{130}}{23}$ | $\sqrt{\frac{91}{18}}$ | $\left(\frac{130}{21}\right)^3$ | (10,13) |
| 2mn-2n | $\frac{\sqrt{143}}{12}$ | $\sqrt{\frac{22}{143}}$ | $\left(\frac{143}{22}\right)^3$ | (11,13) |
| 6mn-4n | 1 | $\sqrt{\frac{24}{169}}$ | $\left(\frac{169}{24}\right)^3$ | (13,13) |

The following table gives details for types of edges, their numbers and the value of $\sigma_i^{'}, \beta_i^{'}, \theta_i^{'}$ of a molecular graph $TiO_2[m,n]$.

According to the definitions of $GA5$, $ABC4$, S-invariants and from Table 2, we desired the following results.

**Theorem 2.2.** *Let $G = TiO_2[m,n]$ nanotubes. Then*

(i) $GA_5(G) = 3m\left(\frac{\sqrt{99}}{5}\right) + n\left(\frac{3\sqrt{3}}{4} + \frac{48\sqrt{2}}{17} + \frac{12\sqrt{10}}{19} + \frac{\sqrt{91}}{5} + \frac{4\sqrt{130}}{23} - \frac{\sqrt{143}}{6} - 4\right) + mn\left(\frac{8\sqrt{30}}{23} + \frac{\sqrt{143}}{6} + 6\right) + \frac{4\sqrt{50}}{15} + \frac{\sqrt{35}}{3}$

(ii) $ABC_4(G) = 2mn\left(2\sqrt{\frac{19}{18}} + \sqrt{\frac{22}{143}} + \sqrt{\frac{24}{169}}\right) + 3m\left(\sqrt{\frac{15}{72}} + 2\sqrt{\frac{2}{7}}\right) + 2n\left(\sqrt{\frac{17}{90}} + 2\sqrt{\frac{20}{117}} + \sqrt{\frac{21}{130}} + \sqrt{\frac{18}{99}} + \sqrt{\frac{91}{18}} - \sqrt{\frac{22}{143}} - \sqrt{\frac{24}{169}}\right) + 2\left(\sqrt{\frac{13}{50}} + \sqrt{\frac{14}{63}}\right)$

(iii) $S(G) = 2mn\left(2\left(\frac{130}{21}\right)^3 + \left(\frac{143}{22}\right)^3 - 2\left(\frac{169}{24}\right)^3\right) + 3m\left(\left(\frac{117}{20}\right)^3 + +2\left(\frac{99}{18}\right)^3\right) + 2n\left(\left(\frac{63}{14}\right)^3 + 2\left(\frac{72}{15}\right)^3 + \left(\frac{90}{17}\right)^3 + \left(\frac{91}{18}\right)^3 + \left(\frac{130}{21}\right)^3 - \left(\frac{143}{22}\right)^3 - 2\left(\frac{169}{24}\right)^3\right) + 2\left(\left(\frac{50}{13}\right)^3 + \left(\frac{7}{2}\right)^3\right)$

## 3. Armchair Polyhex Nanotubes

Let $TUAC_6[m,n]$ denote a class of the armchair polyhex nanotubes, where $m$ and $n$ are the numbers of hexagons in the first row and in the first column of the corresponding 2D-lattice. In the following table gives the Types of edges, their numbers and amounts of $\sigma_i, \beta_i, \theta_i$ of $TUAC_6[m,n]$.

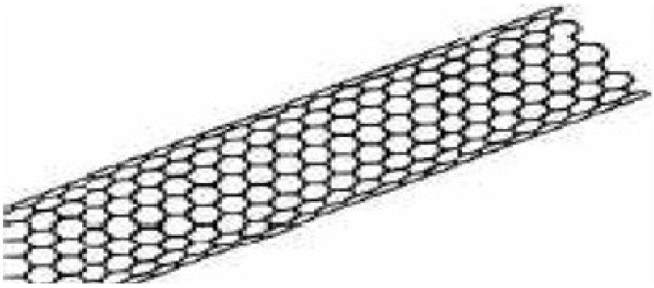

FIGURE 2

TABLE 3

| Number of edges | $\sigma_i$ | $\beta_i$ | $\theta_i$ | Types of edges |
|---|---|---|---|---|
| $2\binom{m}{n}$ | 1 | $\sqrt{\frac{1}{2}}$ | 8 | (2,2) |
| 2m | $\frac{2\sqrt{6}}{5}$ | $\sqrt{\frac{1}{2}}$ | 8 | (3,2) |
| 3mn-m | 1 | $\frac{2}{3}$ | $\frac{729}{64}$ | (3,3) |

TABLE 4. Types of edges, their numbers and amount of $\sigma_i^{'}, \beta_i^{'}, \theta_i^{'}$ of $TUAC_6[m,n]$. Let $G = TUAC_6[m,n]$.

| Number of edges | $\sigma_i^{'}$ | $\beta_i^{'}$ | $\theta_i^{'}$ | Types of edges |
|---|---|---|---|---|
| M | 1 | $\sqrt{\frac{8}{25}}$ | $\left(\frac{25}{8}\right)^3$ | (5,5) |
| 2m | $\frac{4\sqrt{10}}{13}$ | $\sqrt{\frac{11}{40}}$ | $\left(\frac{40}{11}\right)^3$ | (5,8) |
| M | 1 | $\sqrt{\frac{7}{32}}$ | $\left(\frac{64}{14}\right)^3$ | (8,8) |
| 2m | $\frac{12\sqrt{2}}{17}$ | $\sqrt{\frac{15}{72}}$ | $\left(\frac{72}{15}\right)^3$ | (8,9) |
| 3mn-4m | 1 | $\frac{4}{9}$ | $\left(\frac{81}{16}\right)^3$ | (9,9) |

According to the definitions of molecular descriptors and Table 3 and Table 4, we get the following results.

**Theorem 3.1.** *Let* $G = TUAC_6[m,n]$. *Then*

(i) $ABC(G) = m\Big(3\sqrt{\frac{1}{2}} - \frac{2}{3}\Big) + 3mn\left(\frac{2}{3}\right).$

(ii) $GA(G) = 3mn + \frac{4\sqrt{6}}{5}m$ *and*

(iii) $AZI(G) = \left(\frac{807}{64}\right)m + \left(\frac{2187}{64}\right)mn.$

**Theorem 3.2.** *Let* $G = TUAC_6[m,n]$. *Then*

(i) $ABC_4(G) = m\Big(\frac{2\sqrt{2}}{5} + 4\sqrt{\frac{10}{11}} + 8\sqrt{\frac{1}{14}} + 12\sqrt{\frac{2}{15}} - 9\Big) + \frac{27mn}{4}.$

(ii) $GA_5(G) = \Big(3n + \frac{8\sqrt{10}}{13} + \frac{24\sqrt{2}}{17} - 2\Big)m.$

(iii) $S(G) = m\Big(\Big(\frac{25}{8}\Big)^3 + 2\Big(\frac{40}{11}\Big)^3 + \Big(\frac{64}{14}\Big)^3 + 2\Big(\frac{72}{15}\Big)^3 - 4\Big(\frac{81}{16}\Big)^3\Big) + 3mn\Big(\frac{81}{16}\Big)^3.$

## REFERENCES

[1] R. EVARESTOV, Y. F. ZHUKOVSKII, A. V. BANDURA, S. PISKUNOV: *Symmetry and models of single-walled $TiO_2$ nanotubes with rectangular morphology*, Cent. Eur. J. Phys., **9**(2) (2011), 492–501.

[2] M. A. MALIK, M. IMRAN: *On multiple Zagreb index of $TiO_2$ nanotubes*, Acta Chim. Slov., **62**(4) (2015), 973–976.

[3] A. R. ASHRAFI, A. LOGHMAN: *PI index of armchair polyhex Nanotube*, Ars Combinatoria, **80** (2006), 193–199.

[4] A. IRANMANESH, A. R. ASHRAFI: *Balaban index of an armchair polyhex nanotube, $TUC_4C_8(R)$ and $TUC_4C_8(S)$ nanotorus*, J. Comput. Theor. Nanosci., **4**(3) (2007), 514–517.

[5] H. DENG: *The PI Index of $TUAC_6[2p,q]$*, MATCH Commun. Math.Comput. Chem., **55** (2006), 461–476.

[6] M. V. DIUDEA, M. STEFU, B. PARV, P. E. JOHN: *Armchair Polyhex Nanotube*, Croat. Chem. Acta, **77**(1) (2004), 111–115.

[7] M. V. DIUDEA: *Hosoya polynomial In Tori*, MATCH Commun. Math.Comput. Chem., **45** (2002), 109–122.

[8] M. ELIASI, B. TAERI: *Distance in Armchair Polyhex Nanotube*, MATCH Commun. Math. Comput. Chem., **62** (2009), 295–310.

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