

ON SOME DESCRIPTORS OF MOLECULAR GRAPHS

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ABSTRACT. Degree based topological invariants are very important to study the properties of molecular graphs. In this paper, we present some degree based topological indices of copper(II) oxide molecular graph and Polycyclic Aromatic Hydrocarbon.

1. INTRODUCTION

Graph theory is a very powerful area of mathematics that has wide range of applications in many areas of science such as chemistry, biology, computer science, electrical, electronics and other fields. The examination of chemical structural information is made conceivable using molecular descriptors. Chemical graph theory is a branch of mathematical chemistry in which we apply tools of graph theory to model the chemical phenomenon mathematically. Furthermore, it relates to the nontrivial applications of graph theory for solving molecular problems. This theory contributes a prominent role in the field of chemical sciences. Chem-informatics is new subject which is a combination of chemistry, mathematics and information science. Some references are given, which hopefully demonstrate the importance of this field [1–7].

A topological invariant is a mathematical measure which correlates to the chemical structures of any simple finite graph. They play an important role in the study of *QSAR/QSPR*.

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- The sum-connectivity invariant: $\chi_\alpha(\Lambda) = \sum_{uv \in E(\Lambda)} (\tau_G(u) + \tau_G(v))^\alpha$, where α is a real number.
- The geometric-arithmetic invariant: $GA(\Lambda) = \sum_{uv \in E(\Lambda)} \frac{2\sqrt{\tau_G(u)\tau_G(v)}}{\tau_G(u) + \tau_G(v)}$.
- The atom-bond connectivity: $ABC(\Lambda) = \sum_{uv \in E(\Lambda)} \sqrt{\frac{\tau_G(u) + \tau_G(v) - 2}{\tau_G(u)\tau_G(v)}}$.
- The augmented Zagreb invariant: $AZI(\Lambda) = \sum_{uv \in E(\Lambda)} \left(\frac{\tau_G(u)\tau_G(v)}{\tau_G(u) + \tau_G(v) - 2} \right)^3$.
- The inverse sum indeg invariant: $ISI(\Lambda) = \sum_{uv \in E(\Lambda)} \frac{\tau_G(u)\tau_G(v)}{\tau_G(u) + \tau_G(v)}$.
- The symmetric division deg invariant: $SDD(\Lambda) = \sum_{uv \in E(\Lambda)} \frac{\tau_G(u)^2 + \tau_G(v)^2}{\tau_G(u)\tau_G(v)}$.
- The harmonic polynomial: $H(\Lambda, x) = \sum_{uv \in E(\Lambda)} 2x^{\tau_G(u) + \tau_G(v) - 1}$. Note that $\int_0^1 H(\Lambda, x) dx = H(\Lambda)$.

The equivalent definitions of GA invariant, ABC invariant and Augmented Zagreb invariant are defined as follows:

- $GA(\Lambda) = \sum_{i=1}^{|E(\Lambda)|} \sigma_i$, where $\sigma_i = \frac{2\sqrt{\tau(u_i)\tau(v_i)}}{\tau(u_i) + \tau(v_i)}$,
- $ABC(\Lambda) = \sum_{i=1}^{|E(\Lambda)|} \eta_i$, where $\eta_i = \sqrt{\frac{\tau(u_i) + \tau(v_i) - 2}{\tau(u_i)\tau(v_i)}}$, and
- $AZI(\Lambda) = \sum_{i=1}^{|E(\Lambda)|} \theta_i$, where $\theta_i = \left(\frac{\tau(u_i)\tau(v_i)}{\tau(u_i) + \tau(v_i) - 2} \right)^{\frac{1}{3}}$.

Let $S(u_i) = \sum_{v_i \in N(u_i)} \tau_G(v_i)$, where $N(u_i) = \{v_i \in V(\Lambda) | u_i v_i \in E(\Lambda)\}$. The fourth atom bond connectivity invariant, fifth geometric arithmetic invariant and sanku-rati invariant are defined as follows:

- $ABC_4(\Lambda) = \sum_{i=1}^{|E(\Lambda)|} \sigma'_i$, where $\sigma'_i = \frac{2\sqrt{S(u_i)S(v_i)}}{S(u_i) + S(v_i)}$,
- $GA_5(\Lambda) = \sum_{i=1}^{|E(\Lambda)|} \eta'_i$, where $\eta'_i = \sqrt{\frac{S(u_i) + S(v_i) - 2}{S(u_i)S(v_i)}}$, and
- $S(\Lambda) = \sum_{i=1}^{|E(\Lambda)|} \theta'_i$, where $\theta'_i = \left(\frac{S(u_i)S(v_i)}{S(u_i) + S(v_i) - 2} \right)^{\frac{1}{3}}$.

2. MAIN RESULTS

The copper(II) oxide form an inorganic chemical compound CuO . This is an essential mineral found in plants and animals. Copper has enormous applications in medical instruments, drugs, and as a heat conductor, among others. The applications of copper and cupric oxide is given in [8]. The construction of the CuO graph is such that the octagons are connected to each other in columns and rows; the connection between two octagons is achieved by making one $C4$ bond between two octagons. For our convenience, we take m and n as the number of octagons in rows and columns, respectively.

Theorem 2.1. *Let $\Lambda = CuO$ be a copper(II) Oxide graph. Then*

- (i) $\chi_\alpha(\Lambda) = 2mn(5^\alpha + 2(7^\alpha)) + 4m(5^\alpha - 7^\alpha) + 2n(2(4^\alpha + 6^\alpha - 7^\alpha - 5^\alpha)) + 4(4^\alpha - 5^\alpha - 6^\alpha + 7^\alpha)$.
- (ii) $ISI(\Lambda) = 4 \left[\left(\frac{81}{35}\right)mn - \left(\frac{18}{35}\right)m + \left(\frac{2}{105}\right)n - \frac{61}{105} \right]$.
- (iii) $SDD(\Lambda) = \left(\frac{38}{3}\right)mn + \frac{m}{3} + \frac{16}{m} - \frac{7}{3}$.
- (iv) $AZI(\Lambda) = 4 \left[(17.824)mn - (5.824)m + (1,824)n + 5.824 \right]$.
- (v) $GA(\Lambda) = 4mn\left(\frac{\sqrt{6}}{5} + \frac{4\sqrt{3}}{7}\right) + 8m\left(\frac{\sqrt{6}}{5} + \frac{2\sqrt{3}}{7}\right) + 4n\left(1 - \frac{\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - \frac{4\sqrt{3}}{7}\right) + \left(4 - \frac{8\sqrt{6}}{5} - \frac{8\sqrt{2}}{3}\right) + \frac{16\sqrt{3}}{7}$.
- (vi) $ABC(\Lambda) = 2mn\left(\frac{1}{\sqrt{2}} + \sqrt{\frac{5}{3}}\right) + 2m\left(\sqrt{2} - \sqrt{\frac{5}{3}}\right) - 2n\left(\frac{3}{\sqrt{2}} + \sqrt{\frac{5}{3}}\right) + 2\left(\sqrt{\frac{5}{3}} - \sqrt{2}\right)$.

Proof. Let m and n be the number of octagons in rows and columns, respectively. From the structure of CuO , the number of vertices and edges in the graph CuO are $4mn + 3n + m$ and $6mn + 2n$, respectively. From Table 1 and the definitions of indices, we obtain the required result. \square

TABLE 1. Types of edges, their numbers and amount of $\sigma_i, \eta_i, \theta_i, \mu_i, \epsilon_i, \beta_i$ of the molecular graph Cuo .

Number of edges	σ_i	η_i	θ_i	Type of edges	μ_i	ϵ_i	β_i
$4n + 4$	1	$\sqrt{\frac{1}{2}}$	8	(2, 2)	4^α	1	2
$2mn + 4m - 2n - 4$	$\frac{2\sqrt{6}}{5}$	$\sqrt{\frac{1}{2}}$	8	(2, 3)	5^α	$\frac{6}{5}$	$\frac{13}{6}$
$4n - 4$	$\frac{2\sqrt{2}}{3}$	$\sqrt{\frac{1}{2}}$	8	(2, 4)	6^α	$\frac{4}{3}$	$\frac{5}{2}$
$4mn - 4m - 4n + 4$	$\frac{4\sqrt{3}}{7}$	$\sqrt{\frac{5}{12}}$	$\left(\frac{12}{5}\right)^3$	(3, 4)	7^α	$\frac{12}{7}$	$\frac{25}{12}$

By using Theorem 2.1, we obtain the following corollary.

Corollary 2.1. Let $\Lambda = CuO$ be a copper(II) Oxide graph. Then

$$\chi_{\alpha}(\Lambda) = \begin{cases} 38mn - 8m + 2n, & \text{if } \alpha = 1; \\ \frac{2m}{35}(7n + 4) + \frac{1}{105}(193n + 11), & \text{if } \alpha = -1; \\ 2(123mn - 48m - 19n + 8), & \text{if } \alpha = 2; \\ 2\sqrt{5}(mn + m - n - 2) + 4\sqrt{7}(mn - m - n + 1) \\ + 4\sqrt{6}(n - 1) + 8(n + 1), & \text{if } \alpha = \frac{1}{2}; \\ \frac{2}{\sqrt{5}}(mn + m - n - 2) + \frac{4}{\sqrt{7}}(mn - m - n + 1) \\ + \frac{4}{\sqrt{6}}(n - 1) + 2(n + 1), & \text{if } \alpha = -\frac{1}{2}; \end{cases}$$

TABLE 2. Types of edges, their numbers and amount of $\sigma'_i, \eta'_i, \theta'_i$ of the molecular graph Cuo .

Number of edges	σ'_i	η'_i	θ'_i	Type of edges
4	1	$\sqrt{\frac{3}{8}}$	$(\frac{8}{3})^3$	(4,4)
4	$\frac{4\sqrt{5}}{9}$	$\frac{1}{2}\sqrt{\frac{7}{5}}$	$(\frac{20}{7})^3$	(4,5)
$4(n - 1)$	$\frac{2\sqrt{6}}{5}$	$\sqrt{\frac{1}{3}}$	27	(4,6)
4	$\frac{2\sqrt{30}}{11}$	$\sqrt{\frac{3}{10}}$	$(\frac{10}{3})^3$	(5,6)
$6m - 10$	1	$\sqrt{\frac{5}{18}}$	$(\frac{18}{5})^3$	6,6
$2(mn - (m - n) - 1)$	$\frac{\sqrt{60}}{8}$	$\sqrt{\frac{7}{30}}$	$(\frac{30}{7})^3$	(6,10)
$4(n - 1)$	1	$\sqrt{\frac{9}{50}}$	$(\frac{50}{9})^3$	(10,10)
$4(mn - (m + 2n) + 2)$	$\frac{2\sqrt{30}}{11}$	$\sqrt{\frac{1}{6}}$	6^3	(10,12)

Theorem 2.2. Let $\Lambda = CuO$ be a copper(II) Oxide graph. Then

- (i) $GA_5(\Lambda) = mn\left(\frac{\sqrt{60}}{4} + \frac{8\sqrt{30}}{11}\right) - m\left(\frac{\sqrt{60}}{4} + \frac{8\sqrt{30}}{11} - 6\right) + n\left(\frac{\sqrt{60}}{4} + \frac{8\sqrt{6}}{5} - \frac{16\sqrt{30}}{11} + 4\right) + \left(\frac{8\sqrt{30}}{11} - \frac{8\sqrt{6}}{5} + \frac{16\sqrt{30}}{11} - \frac{\sqrt{60}}{4} + 2\sqrt{5} - 10\right).$
- (ii) $ABC_4(\Lambda) = 2mn\left(\sqrt{\frac{7}{30}} + 2\sqrt{\frac{1}{6}}\right) + 2m\left(\sqrt{\frac{5}{2}} - \sqrt{\frac{7}{30}} - 2\sqrt{\frac{1}{6}}\right) + 2n\left(2\sqrt{\frac{1}{3}} - 4\sqrt{\frac{1}{6}} + \sqrt{\frac{7}{30}} + \frac{6}{\sqrt{50}}\right) + 2\left(\sqrt{\frac{3}{2}} + \sqrt{\frac{7}{5}} - \sqrt{\frac{7}{30}} + 2\sqrt{\frac{3}{10}} - 2\sqrt{\frac{1}{3}} - 2\sqrt{\frac{9}{50}} + 4\sqrt{\frac{1}{6}} - 5\sqrt{\frac{5}{18}}\right).$

$$(iii) \ S(\Lambda) = 2mn\left(\left(\frac{30}{7}\right)^3 + 432\right) + 2m\left(3\left(\frac{18}{5}\right)^3 - \left(\frac{30}{7}\right)^3 - 432\right) + 2n\left(\left(\frac{30}{7}\right)^3 + 2\left(\frac{50}{9}\right)^3 - 810\right) + 4\left(\left(\frac{8}{3}\right)^3 + \left(\frac{20}{7}\right)^3 + \left(\frac{10}{3}\right)^3 - \left(\frac{50}{9}\right)^3 + 405\right) - 2\left(\left(\frac{30}{7}\right)^3 + 5\left(\frac{18}{5}\right)^3\right).$$

Proof. According to Table 2 and the definitions of GA_5 , ABC_4 and S -indices, we get the required result. \square

3. POLYCYCLIC AROMATIC HYDROCARBONS

In this section, we discuss on the structures of Polycyclic Aromatic Hydrocarbons, for short PAH_k which play a role in organic materials and medical science. Polycyclic Aromatic Hydrocarbons are a group of more than 100 different chemicals that are formed during the incomplete burning of garbage, gas, oil, coal or other organic materials.

Theorem 3.1. *Let $\Lambda = PAH_k$ be a Polycyclic Aromatic Hydrocarbon. Then*

- (i) $GA_5(\Lambda) = 9k^2 + \left(\frac{6\sqrt{21}}{5} + \frac{9\sqrt{7}}{2} - 15\right)k + \left(12 - \frac{9\sqrt{7}}{2}\right).$
- (ii) $ABC_4(\Lambda) = 4k^2 + \left(4\sqrt{2} - \frac{12\sqrt{2}}{\sqrt{21}} - \frac{20}{3}\right)k + \left(\frac{12\sqrt{3}}{7} - 4\sqrt{2} + \frac{8}{3}\right).$
- (iii) $S(\Lambda) = 9\left(\frac{18}{16}\right)^3 k^2 + \left(\frac{3(21)^3}{256} + \frac{2187}{2} - 15\left(\frac{18}{16}\right)^3\right)k + 6\left(\frac{49}{12}\right)^3 - \frac{2187}{2} + 6\left(\frac{18}{16}\right)^3.$

Proof. By the structure of a graph PAH_k , we have $6k^2 + 6k$ vertices and $9k^2 + 3k$ edges. The following table gives the edge partitions and their invariant values. According to Table 3, we have the required result. \square

TABLE 3. Types of edges, their numbers and amount of $\sigma'_i, \eta'_i, \theta'_i$ of the molecular graph Polycyclic aromatic hydrocarbons

Number of edges	σ'_i	η'_i	θ'_i	Type of edges
$6k$	$\frac{\sqrt{21}}{5}$	$\sqrt{\frac{8}{21}}$	$\left(\frac{21}{8}\right)^3$	(3,7)
6	1	$\frac{2\sqrt{3}}{7}$	$\left(\frac{49}{12}\right)^3$	(7,7)
$12(k-1)$	$\frac{3\sqrt{7}}{8}$	$\frac{\sqrt{2}}{3}$	$\left(\frac{9}{2}\right)^3$	(7,9)
$9k^2 - 15k + 6$	1	$\frac{4}{9}$	$\left(\frac{81}{16}\right)^3$	(9,9)

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