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On Some New Domination Topological Indices of Some Chemical Structures

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Abstract: In medical science, pharmacology, chemical, pharmaceutical properties of molecular structure are essential for drug preparation and design. These properties can be studied by using domination topological indices calculation. In this research work, we establish some new Domination topological properties of levodopa-carbidopa drug given to people with Parkinson's disease.

MSC: 05C69, 05C31.

Keywords: Domination indices, Domination Degree, Carbidopa-Levodopa.

1. Introduction

Chemical graph theory is one of the branches of mathematical chemistry. The importance of chemical graph theory lies in understanding and explaining the nature of the chemical composition, as it was used in organizing the current problem because it determines the arrangement of rules and laws according to a specific system and planning. The atoms are represented as the vertices and the chemical bonds between the atoms are the edges connecting these vertices. Topological indicators are molecular descriptors that describe the composition of chemical structures and help predict some of the chemical and physical properties of these structures. A set $D \subseteq V$ is said to be a dominating set of a graph G, if for any vertex $v \in V - D$ there exists a vertex $u \in D$ such that u and v are adjacent. For more details on topological indices of graph and applications in graphs see [1–7, 21, 22, 24] and for more details on domination in graphs, see [14–16, 20, 25]. A dominating set $D = \{v_1, v_2, ..., v_r\}$ is minimal if $D - v_i$ is not a dominating set [19]. A dominating set of G of minimum cardinality is said to be a minimum dominating set.

Definition 1.1 ([23])**.** *For each vertex $v \in V(G)$, the domination degree denotes by $d_d(v)$ and define as the number of minimal dominating sets of G which contains v.*

In [23] Hanan Ahmed, have introduced new degree-based topological indices called domination Zagreb indices which are based on the domination degree defined as:

$$DM_1(G) = \sum_{v \in V(G)} d_d^2(v),$$

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$$DM_2(G) = \sum_{uv\in E(G)} d_d(u)d_d(v),$$
$$DM_1^*(G) = \sum_{uv\in E(G)} [d_d(u) + d_d(v)].$$

Where $d_d(v)$ is the domination degree of the vertex v. In [23], the total number of minimal dominating sets of G is denoted as $T_m(G)$. The forgotten domination, hyper domination and modified forgotten domination indices of graphs [8] are defined as:

$$DF(G) = \sum_{v\in V(G)} d_d^3(v),$$
$$DH(G) = \sum_{uv\in E(G)} [d_d(u) + d_d(v)]^2,$$
$$DF^*(G) = \sum_{uv\in E(G)} (d_d^2(u) + d_d^2(v)).$$

For more information on topological indices of graph and its applications see [10–13, 17, 18]. In 2022, the authors [2] defined the domination Sombor index as

$$DSO(G) = \sum_{uv\in E(G)} \sqrt{d_d^2(u) + d_d^2(v)} \tag{1}$$

In this paper, we define new domination topological indices as domination Somber index, domination harmonic index, domination inverse sum indeg index, domination atom bound connectivity index, domination geometric arithmetic index, and domination arithmetic geometric index which define as follows:

$$Dh(G) = \sum_{uv\in E(G)} \frac{2}{d_d(u) + d_d(v)} \tag{2}$$
$$DISI(G) = \sum_{uv\in E(G)} \frac{d_d(u)d_d(v)}{d_d(u) + d_d(v)} \tag{3}$$
$$DABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_d(u) + d_d(v) - 2}{d_d(u)d_d(v)}} \tag{4}$$
$$DGA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_d(u)d_d(v)}}{d_d(u) + d_d(v)} \tag{5}$$
$$DAG(G) = \sum_{uv\in E(G)} \frac{d_d(u) + d_d(v)}{2\sqrt{d_d(u)d_d(v)}} \tag{6}$$

2. Results and Discussion

Levodopa was developed over 30 years ago and is often considered the appropriate standard for Parkinson's treatment. levodopa works by crossing the blood-brain barrier, where it is converted to dopamine. The blood enzymes break down most of the levodopa before it reaches the brain. For this reason, levodopa is combined with an enzyme inhibitor called carbidopa. The addition of carbidopa prevents levodopa from being metabolized in the gastrointestinal tract and liver. In this paper, we used the notations $G \cong$ molecular graph of levodopa and $H \cong$ molecular graph of carbidopa.

2.1. Results for Levodopa

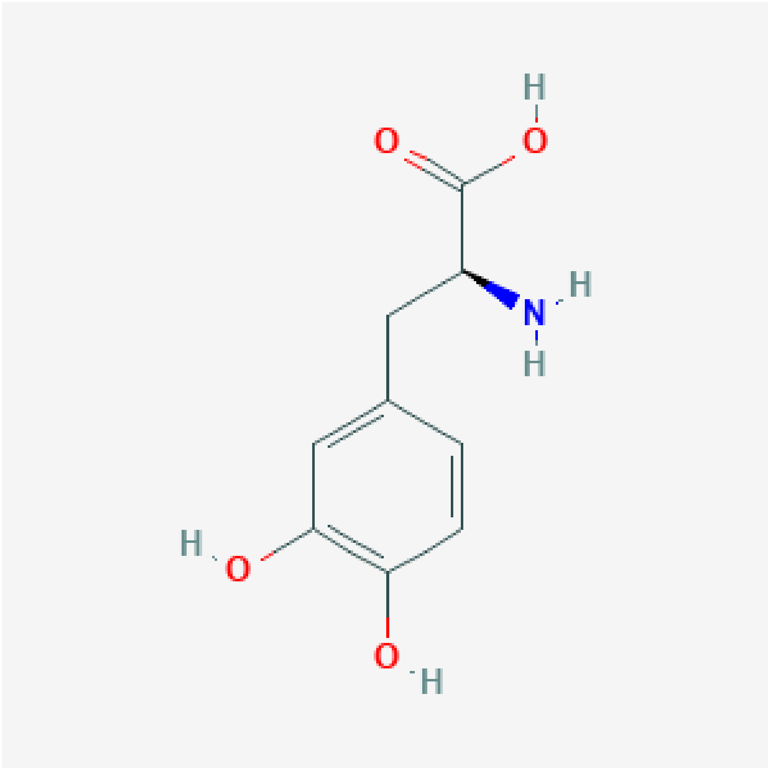

Figure 1. **Chemical structure of Levodopa** $C_9H_{11}NO_4$

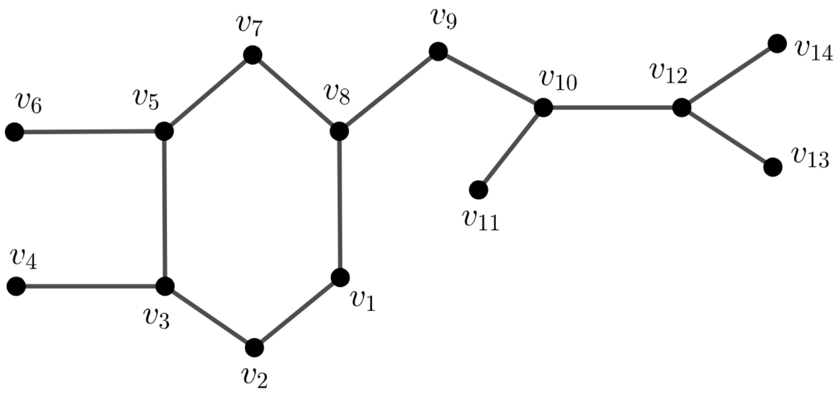

Figure 2. **Molecular graph of Levodopa** $C_9H_{11}NO_4$

Theorem 2.1. *Let G be the molecular graphs of levodopa. Then $T_m(G) = 49$, and there are 6 minimum dominating sets in the molecular graphs of levodopa.*

Proof. Let G be the molecular graph of levodopa $C_9H_{11}NO_4$. The minimal dominating sets of G are:

$D_1 = \{v_1, v_3, v_5, v_{10}, v_{12}\}$, $D_2 = \{v_1, v_4, v_5, v_{10}, v_{12}\}$,

$D_3 = \{v_1, v_3, v_6, v_7, v_{10}, v_{12}\}$, $D_4 = \{v_1, v_4, v_6, v_7, v_{10}, v_{12}\}$,

$D_5 = \{v_3, v_5, v_8, v_{10}, v_{12}\}$, $D_6 = \{v_3, v_6, v_8, v_{10}, v_{12}\}$,

$D_7 = \{v_2, v_4, v_5, v_8, v_{10}, v_{12}\}$, $D_8 = \{v_2, v_4, v_6, v_8, v_{10}, v_{12}\}$,

$D_9 = \{v_2, v_3, v_5, v_7, v_{10}, v_{12}\}$, $D_{10} = \{v_2, v_3, v_6, v_7, v_{10}, v_{12}\}$,

$D_{11} = \{v_2, v_4, v_5, v_7, v_{10}, v_{12}\}$, $D_{12} = \{v_2, v_4, v_6, v_7, v_{10}, v_{12}\}$

$D_{13} = \{v_1, v_3, v_5, v_{10}, v_{13}, v_{14}\}$, $D_{14} = \{v_1, v_4, v_5, v_{10}, v_{13}, v_{14}\}$,

$D_{15} = \{v_1, v_3, v_6, v_7, v_{10}, v_{13}, v_{14}\}$, $D_{16} = \{v_1, v_4, v_6, v_7, v_{10}, v_{13}, v_{14}\}$,

$D_{17} = \{v_3, v_5, v_8, v_{10}, v_{13}, v_{14}\}$, $D_{18} = \{v_3, v_6, v_8, v_{10}, v_{13}, v_{14}\}$,

$D_{19} = \{v_2, v_4, v_5, v_8, v_{10}, v_{13}, v_{14}\}$, $D_{20} = \{v_2, v_4, v_6, v_8, v_{10}, v_{13}, v_{14}\}$,

$D_{21} = \{v_2, v_3, v_5, v_7, v_{10}, v_{13}, v_{14}\}$, $D_{22} = \{v_2, v_3, v_6, v_7, v_{10}, v_{13}, v_{14}\}$,

$D_{23} = \{v_2, v_4, v_5, v_7, v_{10}, v_{13}, v_{14}\}$, $D_{24} = \{v_2, v_4, v_6, v_7, v_{10}, v_{13}, v_{14}\}$

$D_{25} = \{v_1, v_3, v_5, v_9, v_{11}, v_{12}\}$, $D_{26} = \{v_1, v_4, v_5, v_9, v_{11}, v_{12}\}$,

$D_{27} = \{v_1, v_3, v_6, v_7, v_9, v_{11}, v_{12}\}$, $D_{28} = \{v_1, v_4, v_6, v_7, v_9, v_{11}, v_{12}\}$,

$D_{29} = \{v_3, v_5, v_8, v_{11}, v_{12}\}$, $D_{30} = \{v_3, v_6, v_8, v_{11}, v_{12}\}$

$D_{31} = \{v_2, v_4, v_5, v_9, v_{11}, v_{12}\}$, $D_{32} = \{v_2, v_4, v_6, v_8, v_9, v_{11}, v_{12}\}$,

$D_{33} = \{v_2, v_3, v_5, v_9, v_{11}v_{12}\}$, $D_{34} = \{v_2, v_3, v_6, v_7, v_9, v_{11}, v_{12}\}$,

$D_{35} = \{v_2, v_4, v_6, v_7, v_9, v_{11}, v_{12}\}$, $D_{36} = \{v_1, v_3, v_5, v_9, v_{11}, v_{13}, v_{14}\}$,

$D_{37} = \{v_1, v_4, v_5, v_9, v_{11}, v_{13}, v_{14}\}$, $D_{38} = \{v_1, v_3, v_6, v_7, v_9, v_{11}, v_{13}, v_{14}\}$,

$D_{39} = \{v_1, v_4, v_6, v_7, v_9, v_{11}, v_{13}, v_{14}\}$, $D_{40} = \{v_3, v_5, v_8, v_{11}, v_{13}, v_{14}\}$,

$D_{41} = \{v_3, v_6, v_8, v_{11}, v_{13}.v_{14}\}$, $D_{42} = \{v_2, v_4, v_5, v_9, v_{11}, v_{13}, v_{14}\}$

$D_{43} = \{v_2, v_4, v_6, v_8, v_{11}, v_{13}, v_{14}\}$, $D_{44} = \{v_2, v_3, v_5, v_9, v_{11}, v_{13}, v_{14}\}$,

$D_{45} = \{v_2, v_3, v_6, v_7, v_9, v_{11}, v_{13}, v_{14}\}$, $D_{46} = \{v_2, v_4, v_5, v_9, v_{11}, v_{13}, v_{14}\}$,

$D_{47} = \{v_2, v_4, v_6, v_7, v_9, v_{11}, v_{13}, v_{14}\}$, $D_{48} = \{v_2, v_4, v_5, v_8, v_{11}, v_{12}\}$,

$D_{49} = \{v_2, v_4, v_5, v_8, v_{11}, v_{13}, v_{14}\}$

Note that among 49 minimal dominating sets, there are 6 minimum dominating sets. □

From Theorem 2.1, Definition 1.1 we get, if $v_i \in V(G)$ then: $d_d(v_1) = 16$, $d_d(v_2) = 24$, $d_d(v_3) = 24$, $d_d(v_4) = 24$, $d_d(v_5)24$, $d_d(v_6) = 24$, $d_d(v_7) = 20$, $d_d(v_8) = 16$, $d_d(v_9) = 17$, $d_d(v_{10}) = 24$, $d_d(v_{11}) = 24$, $d_d(v_{12}) = 24$, $d_d(v_{13}) = 24$, $d_d(v_{14}) = 24$:

Theorem 2.2. *Let G be the molecular graph of levodopa $C_9H_{11}NO_4$. Then*

(1) $DSO(G) = 432.6104442$

(2) $Dh(G) = \frac{17164488}{28575360}$

(3) $DISI(G) = \frac{101526216}{669735}$

(4) $DABC(G) = 4.186212577$

(5) $DGA(G) = 13.9543214$

(6) $DAG(G) = 14.04637002$

Proof. If G is the molecular graph of levodopa $C_9H_{11}NO_4$, then

(1) $DSO(G) = \sum_{uv\in E(G)} \sqrt{d_d^2(u) + d_d^2(v)} = 8\sqrt{24^2+24^2} + \sqrt{20^2+24^2} + \sqrt{16^2+24^2} + \sqrt{17^2+24^2}$

$+ \sqrt{16^2+16^2} + \sqrt{16^2+17^2} + \sqrt{16^2+20^2}$

$= 192\sqrt{2} + 4\sqrt{61} + 8\sqrt{13} + \sqrt{865} + 16\sqrt{2} + \sqrt{545} + 4\sqrt{41}$

$= 432.6104442$

(2) $Dh(G) = \sum_{uv\in E(G)} \frac{2}{d_d(u)+d_d(v)} = \frac{16}{24+24} + \frac{2}{20+24} + \frac{2}{16+24} + \frac{2}{17+24} + \frac{2}{16+16} + \frac{2}{16+17} + \frac{2}{16+20}$

$= \frac{1}{3} + \frac{1}{22} + \frac{1}{20} + \frac{2}{41} + \frac{1}{16} + \frac{2}{33}$

$= \frac{17164488}{28575360}$

(3) $DISI(G) = \sum_{uv\in E(G)} \frac{d_d(u)d_d(v)}{d_d(u)+d_d(v)} = \frac{8\times 24\times 24}{24+24} + \frac{20\times 24}{20+24} + \frac{16\times 24}{16+24} + \frac{17\times 24}{17+24} + \frac{16\times 16}{16+16} + \frac{16\times 17}{16+17} + \frac{16\times 20}{16+20}$

$= 96 + \frac{120}{11} + \frac{48}{5} + \frac{408}{41} + 8 + \frac{272}{33} + \frac{80}{9}$

$= \frac{101526216}{669735}$

(4) $DABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_d(u)+d_d(v)-2}{d_d(u)d_d(v)}} = 8\sqrt{\frac{24+24-2}{24\times 24}} + \sqrt{\frac{20+24-2}{20\times 24}} + \sqrt{\frac{16+24-2}{16\times 24}}$

$+ \sqrt{\frac{17+24-2}{17\times 24}} + \sqrt{\frac{16+16-2}{16\times 16}} + \sqrt{\frac{16+17-2}{16\times 17}} + \sqrt{\frac{16+20-2}{16\times 20}}$

$= \frac{8\sqrt{46}}{24} + \frac{\sqrt{35}}{20} + \frac{\sqrt{57}}{24} + \frac{\sqrt{442}}{68} + \frac{\sqrt{30}}{16} + \frac{\sqrt{527}}{68} + \frac{\sqrt{170}}{40}$

$= 4.186212577$

(5) $DGA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_d(u)d_d(v)}}{d_d(u)+d_d(v)} = \frac{16\sqrt{24\times 24}}{24+24} + \frac{2\sqrt{20\times 24}}{20+24} + \frac{2\sqrt{16\times 24}}{16+24}$

$+ \frac{2\sqrt{17\times 24}}{17+24} + \frac{2\sqrt{16\times 16}}{16+16} + \frac{2\sqrt{16\times 17}}{16+17} + \frac{2\sqrt{16\times 20}}{16+20}$

$= \frac{384}{48} + \frac{8\sqrt{30}}{44} + \frac{16\sqrt{6}}{40} + \frac{4\sqrt{102}}{41} + \frac{32}{32} + \frac{8\sqrt{17}}{33} + \frac{16\sqrt{5}}{36}$

$= 13.9543214$

(6) $DAG(G) = \sum_{uv\in E(G)} \frac{d_d(u)+d_d(v)}{2\sqrt{d_d(u)d_d(v)}} = \frac{8(24+24)}{2\sqrt{24\times 24}} + \frac{20+24}{2\sqrt{20\times 24}} + \frac{16+24}{2\sqrt{16\times 24}}$

$+ \frac{17+24}{2\sqrt{17\times 24}} + \frac{16+16}{2\sqrt{16\times 16}} + \frac{16+17}{2\sqrt{16\times 17}} + \frac{16+20}{2\sqrt{16\times 20}}$

$= \frac{384}{48} + \frac{44}{8\sqrt{30}} + \frac{40}{16\sqrt{6}} + \frac{41}{4\sqrt{102}} + \frac{32}{32} + \frac{33}{8\sqrt{17}} + \frac{36}{16\sqrt{5}}$

$= 14.04637002$

□

2.2. Results for Carbidopa

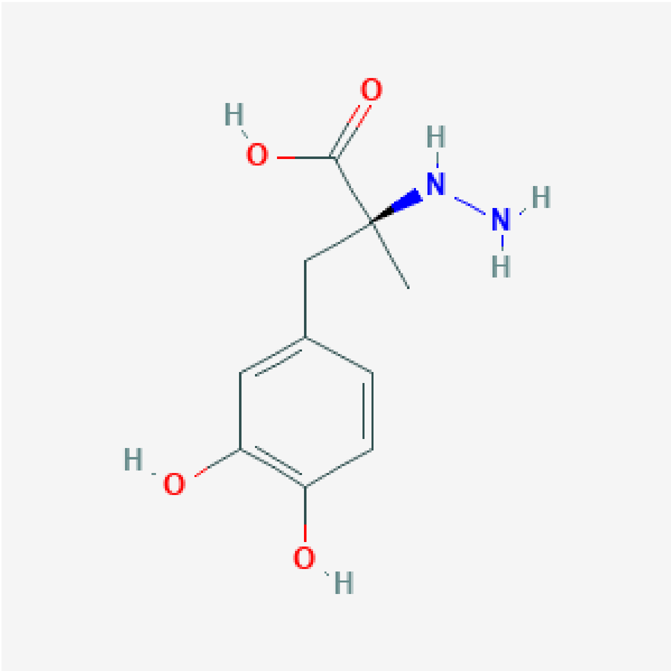

Figure 3. **Chemical structure of Carbidopa** $C_{10}H_{14}N_2O_4$

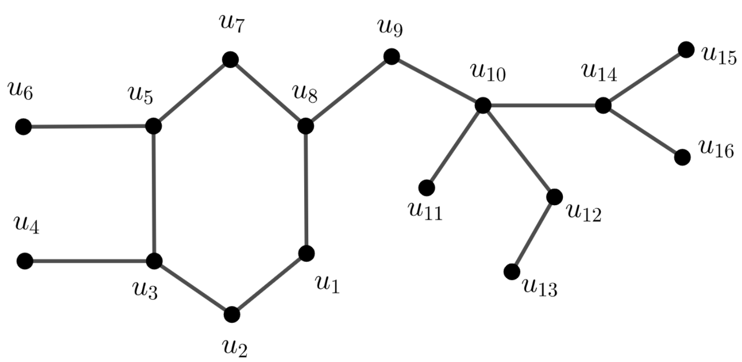

Figure 4. **Molecular graph Carbidopa** $C_{10}H_{14}N_2O_4$

Theorem 2.3. *Let H be the molecular graph of carbidopa $C_{10}H_{14}N_2O_4$. Then $T_m(H) = 96$ and there are 10 minimum dominating sets in the molecular graph carbidopa.*

Proof. Let H be the molecular graph of carbidopa $C_{10}H_{14}N_2O_4$. The minimal dominating sets of H are:

$D_1 = \{u_1, u_3, u_5, u_{10}, u_{12}, u_{14}\}$, $D_2 = \{u_1, u_4, u_5, u_{10}, u_{12}, u_{14}\}$

$D_3 = \{u_1, u_3, u_6, u_7, u_{10}, u_{12}, u_{14}\}$, $D_4 = \{u_1, u_4, u_6, u_7, u_{10}, u_{12}, u_{14}\}$

$D_5 = \{u_3, u_5, u_8, u_{10}, u_{12}, u_{14}\}$, $D_6 = \{u_3, u_6, u_8, u_{10}, u_{12}, u_{14}\}$

$D_7 = \{u_2, u_4, u_5, u_8, u_{10}, u_{12}, u_{14}\}$, $D_8 = \{u_2, u_4, u_6, u_8, u_{10}, u_{12}, u_{14}\}$

$D_9 = \{u_2, u_3, u_5, u_7, u_{10}, u_{12}, u_{14}\}$, $D_{10} = \{u_2, u_3, u_6, u_7, u_{10}, u_{12}, u_{14}\}$

$D_{11} = \{u_2, u_4, u_5, u_7, u_{10}, u_{12}, u_{14}\}$, $D_{12} = \{u_2, u_4, u_6, u_7, u_{10}, u_{12}, u_{14}\}$

$D_{13} = \{u_1, u_3, u_5, u_{10}, u_{12}, u_{15}, u_{16}\}$, $D_{14} = \{u_1, u_4, u_5, u_{10}, u_{12}, u_{15}, u_{16}\}$

$D_{15} = \{u_1, u_3, u_6, u_7, u_{10}, u_{12}, u_{15}, u_{16}\}$, $D_{16} = \{u_1, u_4, u_6, u_7, u_{10}, u_{12}, u_{15}, u_{16}\}$

$D_{17} = \{u_3, u_5, u_8, u_{10}, u_{12}, u_{15}, u_{16}\}$, $D_{18} = \{u_3, u_6, u_8, u_{10}, u_{12}, u_{15}, u_{16}\}$

$D_{19} = \{u_2, u_4, u_5, u_8, u_{10}, u_{12}, u_{15}, u_{16}\}$, $D_{20} = \{u_2, u_4, u_6, u_8, u_{10}, u_{12}, u_{15}, u_{16}\}$

$D_{21} = \{u_2, u_3, u_5, u_7, u_{10}, u_{12}, u_{15}, u_{16}\}$, $D_{22} = \{u_2, u_3, u_6, u_7, u_{10}, u_{12}, u_{15}, u_{16}\}$

$D_{23} = \{u_2, u_4, u_5, u_7, u_{10}, u_{12}, u_{15}, u_{16}\}$, $D_{24} = \{u_2, u_4, u_6, u_7, u_{10}, u_{12}, u_{15}, u_{16}\}$

$D_{25} = \{u_1, u_3, u_5, u_{10}, u_{13}, u_{14}\}$, $D_{26} = \{u_1, u_4, u_5, u_{10}, u_{13}, u_{14}\}$

$D_{27} = \{u_1, u_3, u_6, u_7, u_{10}, u_{13}, u_{14}\}$, $D_{28} = \{u_1, u_4, u_6, u_7, u_{10}, u_{13}, u_{14}\}$

$D_{29} = \{u_3, u_5, u_8, u_{10}, u_{13}, u_{14}\}$, $D_{30} = \{u_3, u_6, u_8, u_{10}, u_{13}, u_{14}\}$

$D_{31} = \{u_2, u_4, u_5, u_8, u_{10}, u_{13}, u_{14}\}$, $D_{32} = \{u_2, u_4, u_6, u_8, u_{10}, u_{13}, u_{14}\}$

$D_{33} = \{u_2, u_3, u_5, u_7, u_{10}, u_{13}, u_{14}\}$, $D_{34} = \{u_2, u_3, u_6, u_7, u_{10}, u_{13}, u_{14}\}$

$D_{35} = \{u_2, u_4, u_5, u_7, u_{10}, u_{13}, u_{14}\}$, $D_{36} = \{u_2, u_4, u_6, u_7, u_{10}, u_{13}, u_{14}\}$

$D_{37} = \{u_1, u_3, u_5, u_{10}, u_{13}, u_{15}, u_{16}\}$, $D_{38} = \{u_1, u_4, u_5, u_{10}, u_{13}, u_{15}, u_{16}\}$

$D_{39} = \{u_1, u_3, u_6, u_7, u_{10}, u_{13}, u_{15}, u_{16}\}$, $D_{40} = \{u_1, u_4, u_6, u_7, u_{10}, u_{13}, u_{15}, u_{16}\}$

$D_{41} = \{u_3, u_5, u_8, u_{10}, u_{13}, u_{15}, u_{16}\}$, $D_{42} = \{u_3, u_6, u_8, u_{10}, u_{13}, u_{15}, u_{16}\}$

$D_{43} = \{u_2, u_4, u_5, u_8, u_{10}, u_{13}, u_{15}, u_{16}\}$, $D_{44} = \{u_2, u_4, u_6, u_8, u_{10}, u_{13}, u_{15}, u_{16}\}$

$D_{45} = \{u_2, u_3, u_5, u_7, u_{10}, u_{13}, u_{15}, u_{16}\}$, $D_{46} = \{u_2, u_3, u_6, u_7, u_{10}, u_{13}, u_{15}, u_{16}\}$

$D_{47} = \{u_2, u_4, u_5, u_7, u_{10}, u_{13}, u_{15}, u_{16}\}$, $D_{48} = \{u_2, u_4, u_6, u_7, u_{10}, u_{13}, u_{15}, u_{16}\}$

$D_{49} = \{u_1, u_3, u_5, u_9, u_{11}, u_{13}, u_{14}\}$, $D_{50} = \{u_1, u_4, u_5, u_9, u_{11}, u_{13}, u_{14}\}$

$D_{51} = \{u_1, u_3, u_6, u_7, u_9, u_{11}, u_{13}, u_{14}\}$, $D_{52} = \{u_1, u_4, u_6, u_7, u_9, u_{11}, u_{13}, u_{14}\}$

$D_{53} = \{u_3, u_5, u_8, u_{11}, u_{13}, u_{14}\}$, $D_{54} = \{u_3, u_6, u_8, u_{11}, u_{13}, u_{14}\}$

$D_{55} = \{u_2, u_4, u_5, u_8, u_{11}, u_{13}, u_{14}\}$, $D_{56} = \{u_2, u_4, u_6, u_8, u_{11}, u_{13}, u_{14}\}$

$D_{57} = \{u_2, u_3, u_5, u_9, u_{11}, u_{13}, u_{14}\}$, $D_{58} = \{u_2, u_3, u_6, u_7, u_9, u_{11}, u_{13}, u_{14}\}$

$D_{59} = \{u_2, u_4, u_5, u_9, u_{11}, u_{13}, u_{14}\}$, $D_{60} = \{u_2, u_4, u_6, u_7, u_9, u_{11}, u_{13}, u_{14}\}$

$D_{61} = \{u_1, u_3, u_5, u_9, u_{11}, u_{13}, u_{15}, u_{16}\}$, $D_{62} = \{u_1, u_4, u_5, u_9, u_{11}, u_{13}, u_{15}, u_{16}\}$

$D_{63} = \{u_1, u_3, u_6, u_7, u_9, u_{11}, u_{13}, u_{15}, u_{16}\}$, $D_{64} = \{u_1, u_4, u_6, u_7, u_9, u_{11}, u_{13}, u_{15}, u_{16}\}$

$D_{65} = \{u_3, u_5, u_8, u_{11}, u_{13}, u_{15}, u_{16}\}$, $D_{66} = \{u_3, u_6, u_8, u_{11}, u_{13}, u_{15}, u_{16}\}$

$D_{67} = \{u_2, u_4, u_5, u_8, u_{11}, u_{13}, u_{15}, u_{16}\}$, $D_{68} = \{u_2, u_4, u_6, u_8, u_{11}, u_{13}, u_{15}, u_{16}\}$

$D_{69} = \{u_2, u_3, u_5, u_9, u_{11}, u_{13}, u_{15}, u_{16}\}$, $D_{70} = \{u_2, u_3, u_6, u_7, u_9, u_{11}, u_{13}, u_{15}, u_{16}\}$

$D_{71} = \{u_2, u_4, u_5, u_9, u_{11}, u_{13}, u_{15}, u_{16}\}$, $D_{72} = \{u_2, u_4, u_6, u_7, u_9, u_{11}, u_{13}, u_{15}, u_{16}\}$

$D_{73} = \{u_1, u_3, u_5, u_9, u_{11}, u_{12}, u_{14}\}$, $D_{74} = \{u_1, u_4, u_5, u_9, u_{11}, u_{12}, u_{14}\}$

$D_{75} = \{u_1, u_3, u_6, u_7, u_9, u_{11}, u_{12}, u_{14}\}$, $D_{76} = \{u_1, u_4, u_6, u_7, u_9, u_{11}, u_{12}, u_{14}\}$

$D_{77} = \{u_3, u_5, u_8, u_{11}, u_{12}, u_{14}\}$, $D_{78} = \{u_3, u_6, u_8, u_{11}, u_{12}, u_{14}\}$

$D_{79} = \{u_2, u_4, u_5, u_8, u_{11}, u_{12}, u_{14}\}$, $D_{80} = \{u_2, u_4, u_6, u_8, u_{11}, u_{12}, u_{14}\}$

$D_{81} = \{u_2, u_3, u_5, u_9, u_{11}, u_{12}, u_{14}\}$, $D_{82} = \{u_2, u_3, u_6, u_7, u_9, u_{11}, u_{12}, u_{14}\}$

$D_{83} = \{u_2, u_4, u_5, u_9, u_{11}, u_{12}, u_{14}\}$, $D_{84} = \{u_2, u_4, u_6, u_7, u_9, u_{11}, u_{12}, u_{14}\}$

$D_{85} = \{u_1, u_3, u_5, u_9, u_{11}, u_{12}, u_{15}, u_{16}\}$, $D_{86} = \{u_1, u_4, u_5, u_9, u_{11}, u_{12}, u_{15}, u_{16}\}$

$D_{87} = \{u_1, u_3, u_6, u_7, u_9, u_{11}, u_{12}, u_{15}, u_{16}\}$, $D_{88} = \{u_1, u_4, u_6, u_7, u_9, u_{11}, u_{12}, u_{15}, u_{16}\}$

$D_{89} = \{u_3, u_5, u_8, u_{11}, u_{12}, u_{15}, u_{16}\}$, $D_{90} = \{u_3, u_6, u_8, u_{11}, u_{12}, u_{15}, u_{16}\}$

$D_{91} = \{u_2, u_4, u_5, u_8, u_{11}, u_{12}, u_{15}, u_{16}\}$, $D_{92} = \{u_2, u_4, u_6, u_8, u_{11}, u_{12}, u_{15}, u_{16}\}$

$D_{93} = \{u_2, u_3, u_5, u_9, u_{11}, u_{12}, u_{15}, u_{16}\}$, $D_{94} = \{u_2, u_3, u_6, u_7, u_9, u_{11}, u_{12}, u_{15}, u_{16}\}$

$D_{95} = \{u_2, u_4, u_5, u_9, u_{11}, u_{12}, u_{15}, u_{16}\}$, $D_{96} = \{u_2, u_4, u_6, u_7, u_9, u_{11}, u_{12}, u_{15}, u_{16}\}$

Note that among 96 minimal dominating sets, there are 10 minimum dominating sets. □

From Theorem 2.3, Definition 1.1 we get, if $u_i \in V(H)$ then: $d_d(u_1) = 32$, $d_d(u_2) = 48$, $d_d(u_3) = 48$, $d_d(u_4) = 48$, $d_d(u_5) = 48$, $d_d(u_6) = 48$, $d_d(u_7) = 40$, $d_d(u_8) = 32$, $d_d(u_9) = 32$, $d_d(u_{10}) = 48$, $d_d(u_{11}) = 48$, $d_d(u_{12}) = 48$, $d_d(u_{13}) = 48$, $d_d(u_{14}) = 48$, $d_d(u_{15}) = 48$, $d_d(u_{16}) = 48$:

Theorem 2.4. *Let H be the molecular graph of carbidopa $C_{10}H_{14}N_2O_4$. Then*

(1) $DSO(H) = 999.9723364$

(2) $Dh(H) = \frac{18304320}{49420800}$

(3) $DISI(H) = \frac{961360}{2925}$

(4) $DABC(H) = 3.404558732$

(5) $DGA(H) = 16.17032432$

(6) $DAG(H) = 2.938183971$

Proof. If H be the molecular graph of carbidopa $C_{10}H_{14}N_2O_4$, then

(1) $$DSO(H) = \sum_{uv\in E(G)} \sqrt{d_d^2(u) + d_d^2(v)} = 10\sqrt{48^2 + 48^2} + 2\sqrt{32^2 + 48^2} + 2\sqrt{33^2 + 32^2} + \sqrt{32^2 + 40^2} + \sqrt{40^2 + 48^2}$$
$$= 480\sqrt{2} + 32\sqrt{13} + 2\sqrt{2119} + 8\sqrt{41} + 8\sqrt{61}$$
$$= 999.9723364$$

(2) $$Dh(H) = \sum_{uv\in E(G)} \frac{2}{d_d(u) + d_d(v)} = \frac{2(10)}{48 + 48} + \frac{2(2)}{32 + 48} + \frac{2(2)}{32 + 32} + \frac{2}{32 + 40} + \frac{2}{40 + 48}$$
$$= \frac{5}{24} + \frac{1}{20} + \frac{4}{65} + \frac{1}{36} + \frac{1}{44}$$
$$= \frac{18304320}{49420800}$$

(3) $$DISI(H) = \sum_{uv\in E(G)} \frac{d_d(u)d_d(v)}{d_d(u) + d_d(v)} = \frac{10 \times 48 \times 48}{48 + 48} + \frac{2 \times 32 \times 48}{32 + 48} + \frac{2 \times 33 \times 32}{33 + 32} + \frac{32 \times 40}{32 + 40} + \frac{40 \times 48}{40 + 48}$$
$$= 240 + \frac{192}{5} + \frac{2112}{65} + \frac{160}{9}$$
$$= \frac{961360}{2925}$$

(4) $$DABC(H) = \sum_{uv\in E(G)} \sqrt{\frac{d_d(u) + d_d(v) - 2}{d_d(u)d_d(v)}} = 10\sqrt{\frac{48 + 48 - 2}{48 \times 48}} + 2\sqrt{\frac{32 + 48 - 2}{32 \times 48}}$$
$$+ 2\sqrt{\frac{33 + 32 - 2}{33 \times 32}} + \sqrt{\frac{32 + 40 - 2}{32 \times 40}} + \sqrt{\frac{40 + 48 - 2}{40 \times 48}}$$
$$= \frac{10\sqrt{94}}{48} + \frac{2\sqrt{13}}{16} + \frac{2\sqrt{462}}{88} + \frac{\sqrt{14}}{16} + \sqrt{\frac{86}{1920}}$$
$$= 3.404558732$$

(5) $DGA(H) = \sum_{uv\in E(G)} \frac{2\sqrt{d_d(d)d_d(v)}}{d_d(u)+d_d(v)} = \frac{20\sqrt{48\times 48}}{48+48} + \frac{4\sqrt{32\times 48}}{32+48} + \frac{4\sqrt{33+32}}{33\times 32} + \frac{2\sqrt{32\times 40}}{32+40} + \frac{2\sqrt{40\times 48}}{40+48}$

$= \frac{960}{96} + \frac{64\sqrt{6}}{80} + \frac{16\sqrt{66}}{65} + \frac{32\sqrt{5}}{72} + \frac{16\sqrt{30}}{72}$

$= 16.17032432$

(6) $DAG(H) = \sum_{uv\in E(G)} \frac{d_d(u)+d_d(v)}{2\sqrt{d_d(u)d_d(v)}} = \frac{48+48}{20\sqrt{48\times 48}} + \frac{32+48}{4\sqrt{32\times 48}} + \frac{33+32}{4\sqrt{33\times 32}} + \frac{32+40}{2\sqrt{32\times 40}} + \frac{40+48}{2\sqrt{40\times 48}}$

$= \frac{96}{960} + \frac{80}{64\sqrt{6}} + \frac{65}{16\sqrt{66}} + \frac{72}{32\sqrt{5}} + \frac{72}{16\sqrt{30}}$

$= 2.938183971$

□

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