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FULL PAPER

Domination version: Sombor index of graphs and its significance in predicting physicochemical properties of butane derivatives

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In graph theory, topological indices and domination parameters are essential topics. A dominating set for a graph G=(V(G),E(G)) is a subset D of V(G) such that every vertex not in D is adjacent to at least one vertex of D introduced novel topological indices known as domination topological indices. In this research work, we found exact values to determine Sombor index of some families of graphs including the join and corona product. Some bounds for these new topological indices were also found. Likewise, we defined the significance of the Sombor index in predicting the physicochemical properties of butane derivatives.

KEYWORDS

Domination topological indices; domination Sombor index; graph operation; QSPR analysis; butane derivatives.

Introduction

Mathematics, chemical graph theory is one of the important branch which is combines with graph theory and chemistry. Graph theory is used to mathematically model molecules to gain insight into the physical properties such as boiling point, melting point, density, and many more chemical compounds, are related to the geometric structure of the compound. Chemical graph theory, which deals with the non-trivial applications of graph theory to solve molecular problems [7]. Topological indices are the most significant molecular descriptor, and it is a mathematical formula that can be applied to any graphs which are related to some chemical components. Topological indices have very important and huge applications (for more details, [6,8,16,21-25,27-38]). Molecular descriptors play a significant role in chemical graph theory. Now a days, there are numerous topological indices some of which are applied to the physiochemical properties of chemical compounds.

Consider G is a graph with no loops and no multiple edges. In G, $V(G)$ is the vertex set and $E(G)$ is the edge set. The vertex of the graph corresponds to an atom, while the edge represents the chemical bond of molecules. The vertex v in G of order n is said to be full degree if d(v)=n-1. A vertex subset D is said to be dominating set such that every vertex v ($v \notin D$) is adjacent to at least one vertex of D. If $D - v$ ($v \in D$) is not a dominating set, then it is called a minimal dominating set and the cardinality of minimum dominating set is called domination number, denoted by $\gamma(G)$ [12]. For more details about domination in the graph, [13,14,18,20]. Hanan Ahmed *et al.* [11] introduced a new degree based on a minimal dominating set, denoted by $d_d(v)$, which is defined as the number of minimal dominating set containing v. We use the

notation $T_m(G)$ which indicates the total number of minimal dominating set of G. For more details regarding domination topological indices of some families of standard graph and graph operations. we refer to study [11]. Likewise, for applications of domination topological indices readers can refer [2,3,4].

Definition 1.1 [4] Let G be a simple, connected graph. Then,

1. The first, the second domination Zagreb, and modified first domination Zagreb indices are defined by:

$$DM_1(G) = \dot{\sum_{u\in V(G)}} d_{d_G}^2(u),$$

$$DM_2(G) = \dot{\sum_{uv\in E(G)}} d_{d_G}(u)d_{d_G}(v),$$

$$DM_1^*(G) = \dot{\sum_{uv\in E(G)}} (d_{d_G}(u) + d_{d_G}(v)).$$

2. The forgotten domination, hyper domination, and modified forgotten domination indices of graphs are defined as follow:

$$DF(G) = \dot{\sum_{u\in V(G)}} d_{d_G}^3(u),$$

$$DH(G) = \dot{\sum_{uv\in E(G)}} [d_{d_G}(u) + d_{d_G}(v)]^2,$$

$$DF^*(G) = \dot{\sum_{uv\in E(G)}} (d_{d_G}^2(u) + d_{d_G}^2(v)).$$

Definition 1.2 [18] Sombor index of graph G is one of the topological index which is defined as:

$$SO(G) = \dot{\sum_{uv\in E(G)}} \sqrt{d_G^2(u) + d_G^2(v)}.$$

In this paper, we introduced new topological indices defined on domination degree named as domination Sombor index defined as:

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

Domination Sombor index of graphs

Definition 2.1 Let G be a simple connected graph. Then, the domination Sombor index is defined as:

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

Proposition 2.2

1. Let $G \cong S_{r+1}$ with $d_d(v) = 1$. Then, $DSO(G) = r\sqrt{2}$.
2. Let $G \cong K_r$, having $d_d(v) = 1$. Then, $DSO(G) = \frac{r(r-1)}{2}\sqrt{2}$.
3. Let $G \cong S_{r+1,s+1}$ with $d_d(v) = 2$. Then, $DSO(G) = 2(r+s+1)\sqrt{2}$.
4. Let $G \cong K_{r,s}, r, s \geq 2$ with $d_d(v) = \begin{cases} r+1; \\ s+1. \end{cases}$ for all $v \in V(G)$. Then $DSO(G) = rs\sqrt{r^2+s^2+2(r+s+1)}$.
5. Let $G \cong \overline{K}_{r,s}$, with $d_{d_{\overline{K}_{r,s}}}(v) = d_{K_{r,s}}(v)$. Then, $DSO(G) = \frac{rs}{2}(r+s-2)\sqrt{2}$.

The Windmill graph Wd_r^s is an undirected graph constructed for $r \geq 2$ and $s \geq 2$ by s copies of the complete graph K_r at a shared universal vertex [5].

Lemma 2.3 [11] Let G be the Windmill graph Wd_r^s. Then,

$$d_d(v) = \begin{cases} 1;\ if\ v\ is\ in\ center; \\ (r-1)^{(s-1)};\ \text{otherwise.} \end{cases}$$

Theorem 2.4 *Let $G \cong Wd_r^s$. Then,*

$$DSO(G) = s(r-1)\left[\sqrt{1+(r-1)^{2(s-1)}}\right] + \left[\frac{sr(r-1)}{2} - s(r-1)\right](r-1)^{(s-1)}\sqrt{2}.$$

Proof. In Wd_r^s, there are two sets of edges. Let E_1 be the set of all edges which are incident with the center vertex and E_2 be the set of all edges of the complete graph. Then,

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

$$= \dot{\sum_{uv\in E_1(G)}} \sqrt{d_d^2(u) + d_d^2(v)} + \dot{\sum_{uv\in E_2(G)}} \sqrt{d_d^2(u) + d_d^2(v)}$$
$$= s(r-1)\left[\sqrt{1^2 + [(r-1)^{(s-1)}]^2}\right] + \left(\frac{sr(r-1)}{2} - s(r-1)\right)\sqrt{[(r-1)^{(s-1)}]^2 + [(r-1)^{(s-1)}]^2}$$
$$= s(r-1)\left[\sqrt{1 + (r-1)^{2(s-1)}}\right] + [\frac{sr(r-1)}{2} - s(r-1)](r-1)^{(s-1)}\sqrt{2}.$$

The book graph B_r, $r \geq 3$ is a cartesian product of star S_{r+1} and path P_1 [5].

Lemma 2.5 [11] If $G \cong B_r$, $r \geq 3$ with $T_m(B_r) = 2^r + 3$, then

$$d_d(v) = \begin{cases} 3, \text{v is center vertex;} \\ 2^{r-1} + 1, otherwise. \end{cases}$$

Theorem 2.6 If $G \cong B_r$ with $r \geq 3$, then

$$DSO(G) = \sqrt{18} + 2r\sqrt{10 + 2^{2(r-1)} + 2^r} + r(2^{r-1} + 1)\sqrt{2}.$$

Proof. Note that here there are three types of edge sets. These are as follow:
$E_1 = \{uv \in E(G): d_d(u) = d_d(v) = 3\}$,
$E_2 = \{uv \in E(G): d_d(u) = 3, d_d(v) = 2^{r-1} + 1\}$,
$E_3 = \{uv \in E(G): d_d(u) = d_d(v) = 2^{r-1} + 1\}$ and $|E_1| = 1, |E_2| = 2r, |E_3| = r$.
So, by using definition of domination Sombor index, we get the results.

Definition 2.7 [11] If the domination degree of all vertices is of G equal to k, then the graph G is said to be k-domination regular graph.

Proposition 2.8 Suppose G is a k-domination regular graph with n vertices and m edges, then
$DSO(G) = mk\sqrt{2}$.

Proposition 2.9 If $G \cong K_{r_1, r_2, \ldots, r_k}$, with $r_1 \geq 2, r_2 \geq 2, \ldots, r_k \geq 2$, then

$$DSO(G) = \dot{\sum_{1\leq l<k}} r_l r_k \sqrt{\begin{matrix}[1 + (\sum_{i=1}^{k} r_i) - r_l]^2 \\ +[1 + (\sum_{i=1}^{k} r_i) - r_k]^2\end{matrix}}$$

Proof. We have $d_d(v) = d(v) + 1$ and $|E(G)| = T_m(G) - k$. By using definition of domination Sombor index, we obtain the required result.

Lemma 2.10 [5] Let G be a Healthy spider graph with 2n + 1 vertices and 2n edges, then $d_d(v) = 1$, for all $v \in V(G)$ and $T_m(G) = 2$.

Theorem 2.11 Let G be a Healthy spider graph with 2n + 1 vertices and 2n edges. Then,
$DSO(G) = 2n\sqrt{2}$.
Proof. By using Proposition 2.8.

Lemma 2.12 [11] Let G be a graph with r vertices and s edges. K_{n_2} be a complete graph. If $H \cong GoK_{n_2}$, then $d_d(v) = (n_2 + 1)^{r-1}$.

Proposition 2.13 If G be a connected graph with r vertices and s edges. Let $H \cong GoK_{n_2}$. Then

$$DSO(H) = \frac{1}{2}(2s + rn_2^2 + rn_2)(n_2 + 1)^{r-1}\sqrt{2}.$$

Proof. Note that, in K_{n_2} there are $\frac{n_2(n_2-1)}{2}$ edges so, there are $\frac{1}{2}(2s + rn_2^2 + rn_2)$ edges in the graph H. Hence,

$$DSO(H) = \dot{\sum_{uv\in E(G)}} \sqrt{d_d^2(u) + d_d^2(v)} = \frac{1}{2}(2s + rn_2^2 + rn_2)(n_2 + 1)^{r-1}\sqrt{2}.$$

Lemma 2.14 *[11] Let* $H \cong GoK_{n_2}$. Then, $d_d(v) = T_m(H) - 2^{r-1}$, *for all* $v \in H$.

Proposition 2.15 If $H \cong GoK_{n_2}$, then
$DSO(H) = (s + rn_2)(T_m(H) - 2^{r-1})\sqrt{2}$.
Proof. By Definition 2.1, and Lemma 2.14, we get the result.

Lemma 2.16 [11] Let G_1 and G_2 be any non-complete graphs with $r_1$and r_2 vertices, respectively, such that no vertex of G_1 and G_2 of a full degree. *Then,* $T_m(G_1 + G_2) = T_m(G_1) + T_m(G_2) + r_1 r_2$, *and*

$$d_{d_{G_1+G_2}}(v) = \begin{cases} d_{d_{G_1}}(v) + r_2, if\, v \in V(G_1); \\ d_{d_{G_2}}(v) + r_1, if\, v \in V(G_2). \end{cases}$$

Theorem 2.17 *If* $G_1 = (r_1 + s_1)$, $G_2 = (r_2 + s_2)$ be any two non complete graphs, , such that no vertex of G_1 and G_2 of a full degree and $G \cong G_1 + G_2$, then

$$DSO(G) = \sqrt{DF^*(G_1) + 2r_2\left(r_2 + DM_1{}^*(G_1)\right)} + \sqrt{DF^*(G_2) + 2r_1\left(r_1 + DM_1{}^*(G_2)\right)} + \sqrt{\begin{matrix} DM_1(G_1) + DM_1(G_2) \\ +r_1\left(r_1 + 2\rho(G_1)\right) + r_2\left(r_2 + 2\rho(G_2)\right) \end{matrix}}$$

Where, $\rho(G) = \sum_{v \in G} d_d(v)$, for all $v \in G$.

Proof. Given, $G \cong G_1 + G_2$ with
$|V(G)| = |V(G_1)| + |V(G_2)|$ and
$|E(G)| = |E(G_1)| + |E(G_2)| \cup uv: u \in V(G_1), v \in V(G_2)$.

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

$$= \dot{\sum_{uv \in E(G_1)}} \sqrt{d_d^2(u) + d_d^2(v)} + \dot{\sum_{uv \in E(G_2)}} \sqrt{d_d^2(u) + d_d^2(v)} + \dot{\sum_{u \in E(G_1), v \in E(G_2)}} \sqrt{d_d^2(u) + d_d^2(v)}$$

$$= \sqrt{\begin{matrix} (d_{d_{G_1}}(u))^2 + (d_{d_{G_1}}(v))^2 + 2r_2^2 \\ +2r_2(d_{d_{G_1}}(u) + d_{d_{G_1}}(v)) \end{matrix}} + \sqrt{\begin{matrix} (d_{d_{G_2}}(u))^2 + (d_{d_{G_2}}(v))^2 + 2r_1^2 \\ +2r_1(d_{d_{G_2}}(u) + d_{d_{G_2}}(v)) \end{matrix}} + \sqrt{\begin{matrix} (d_{d_{G_2}}(u))^2 + (d_{d_{G_2}}(v))^2 + r_1^2 + r_2^2 \\ +2r_2(r_2 d_{d_{G_1}}(u) + r_1 d_{d_{G_2}}(v)) \end{matrix}}$$

$$= \sqrt{DF^*(G_1) + 2r_2\left(r_2 + DM_1{}^*(G_1)\right)} + \sqrt{DF^*(G_2) + 2r_1\left(r_1 + DM_1{}^*(G_2)\right)} + \sqrt{\begin{matrix} DM_1(G_1) + DM_1(G_2) \\ +r_1\left(r_1 + 2\rho(G_1)\right) + r_2\left(r_2 + 2\rho(G_2)\right) \end{matrix}}$$

Some bounds of domination Sombor index

Theorem 3.1 If G = (n, m) be any connected graph for n > 2 and m > 2, then
DSO(G) > ρ(G).

Proof. Consider G is a connected graph with $n > 2$, $m > 2$ and $T_m(G)$ is the total number of domination sets.

We know that $\rho(G) = \sum_{v \in V(G)} d_d(G)$.

We have

$$DSO(G) = \dot{\sum_{uv \in E(G)}} \sqrt{d_d^2(u) + d_d^2(v)} > \dot{\sum_{u \in E(G)}} \sqrt{d_d^2(u)} > \dot{\sum_{u \in E(G)}} d_d(u) = \rho(G).$$

Hence, the result is obtained.

Theorem 3.2 Let G be a k-domination regular graph. Then, $n < DSO(G) < nm$.

Proof. For k-domination regular graph $G = (n, m)$, we have
Since $k < n$ and $n < DSO(G)$, and
$DSO(G) = mk\sqrt{2} < nm\sqrt{2} < nm$
Hence, $n < DSO(G) < nm$.

Theorem 3.3 For a connected graph G of order n and size m, $\sqrt{2}DSO(G) = n(n-1)$ if and only if G is complete.

Proof. Since complete graph G has $\frac{n(n-1)}{2}$ edges and G is 1-domination regular graph. By using Proposition 2.8, we get the results.
Conversely, Since G is connected graph and we have:

$$\sqrt{2}DSO(G) = n(n-1)$$

$$DSO(G) = \frac{n(n-1)}{2}\sqrt{2}$$

By comparing these results, we can say that G is complete graph.

Observation 3.4 $DSO(G) = \sqrt{2}$ if and only if $G = P_2$.

The significance of the Sombor index in predicting the physic-chemical properties of butane derivatives

Quantitative structure-property relationships (QSPR) remain the focus of many studies

aimed at the modeling and prediction of physicochemical and biological properties of molecules. A powerful tool to help in this task is chemometrics, which uses statistical and mathematical methods to extract maximum information from a data set. QSPR uses chemometric methods to describe how a given physicochemical property varies as a function of molecular descriptors describing the chemical structure of the molecule. Thus, it is possible to replace costly biological tests or experiments of a given physicochemical property with calculated descriptors, which can, in turn, be used to predict the responses of interest for new compounds. The basic strategy of QSPR is to find an optimum quantitative relationship, which can be used for the prediction of the properties of compounds, including those unmeasured. It is obvious that the performance of QSPR model mostly depends on the parameters used to describe the molecular structure. Many efforts have been made to develop alternative molecular descriptors which can be derived by using only the information encoded in the chemical structure. Much attention has been concentrated on "topological indices" derived from the connectivity and composition of a molecule which has made significant contributions in QSPR studies. The topological index has advantages of simplicity and quick speed of computation and thus, is of high singificance for the scientists.

In this section, we are going to discuss the QSPR analysis of domination topological indices.

Furthermore, we show that the characteristics have a good correlation with the physicochemical characteristics of butane derivatives, as represented in Table 1. The exact values of domination topological indices of butane derivatives are listed in Table 2.

TABLE 1 Physiochemical properties of butane derivatives

Name of Chemical Compounds	S.T.	Complexity	H.A.C	Density	Refraction Index
1,4-Butanedithiol	31.1	17.5	6	1.03	1.51
-Butanone	22.9	38.5	5	8.32	1.37
1,3-Butanediol	34.9	28.7	6	9.96	1.44
Butane dinitrile	40.7	92	6	1.01	1.42
Butanediamide	53	96.6	8	1.18	1.49
Butane-1-sulfonamide	41.9	133	8	1.15	1.47
1-Butanethiol	24.8	13.1	5	8.5	1.44
1,4-Diamonobutane	35.8	17.5	6	8.65	1.46
Butane-1,4-disulfonic acid	77.9	266	12	1.66	1.54
Butyraldehyde	23.1	24.8	5	8.18	1.37
2,3-Butanedione	27.3	71.5	6	9.75	1.38
1-Butanesulfonyl chloride	36.4	133	8	1.26	1.45

TABLE 2 Exact values of domination topological indices of butane derivatives

No.	Chemical Compounds	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO
1	1,4-Butanedithiol	68	51	32	236	206	104	22.73
2	2-Butanone	20	16	16	40	64	32	11.31
3	1,3-Butanediol	21	16	18	41	66	34	12.96
4	Butane dinitrile	68	51	32	236	206	104	22.73
5	Butanediamide	52	36	32	140	148	76	22.91
6	Butane-1-sulfonamide	100	75	46	364	304	154	32.73
7	1-Butanethiol	17	12	14	33	50	26	10.13
8	1,4-Diamonobutane	68	51	32	236	206	104	22.73
9	Butane-1,4-disulfonic acid	76	71	60	232	334	192	45.65
10	Butyraldehyde	17	12	14	33	50	26	10.13
11	2,3-Butanedione	24	20	20	48	80	40	14.14
12	1-Butanesulfonyl chloride	100	75	46	364	304	154	32.73

In this study, we use the non-linear regression analysis defined as:$log(z_1) = A + B\ log(z)$...(1), where z_1 is the physical and chemical properties of butane derivatives and z_2 represents the domination topological indices. We used R-software to calculate the values of five physiochemical properties of butane derivatives. By using Equation (1), we can obtain different non-linear models for the domination topological indices as follows:

1- The first domination Zagreb index

$$log(ST) = 2.3 + 0.3\ log(DM_1)$$
$$log(Complexity) = 1.02 + 0.8\ log(DM_1)$$
$$log(H.A.C) = 0.9 + 0.2\ log(DM_1)$$
$$log(Density) = 5.7 - 1.2\ log(DM_1)$$
$$log(Index\ of\ Refraction) = 0.2 + 0.03\ log(DM_1).$$

2- The second domination Zagreb index

$$log(ST) = 2.3 + 0.4\ log(DM_2)$$
$$log(Complexity) = 1.1 + 0.8\ log(DM_2)$$
$$log(H.A.C) = 0.9 + 0.3\ log(DM_2)$$
$$log(Density) = 5.2 - 1.1\ log(DM_2)$$
$$log(Index\ of\ Refraction) = 0.2 + 0.04\ log(DM_2).$$

3- Modified first domination Zagreb index

$$log(ST) = 1.5 + 0.6\ log(DM_1^*)$$
$$log(Complexity) = -0.7 + 1.4\ log(DM_1^*)$$
$$log(H.A.C) = 0.36 + 0.4\ log(DM_1^*)$$
$$log(Density) = 6.6 - 1.6\ log(DM_1^*)$$
$$log(Index\ of\ Refraction) = 0.18 + 0.03\ log(DM_1^*).$$

Now the predicted values of physiochemical properties are given in Tables 3, 4, and 5.

4- Forgotten domination index

$$log(ST) = 2.4 + 0.2\ log(DF)$$
$$log(Complexity) = 1.4 + 0.5\ log(DF)$$
$$log(H.A.C) = 1.05 + 0.2\ log(DF)$$
$$log(Density) = 5.2 - 0.8\ log(DF_1)$$
$$log(Index\ of\ Refraction) = 0.2 + 0.02\ log(DF).$$

5- Hyper domination index

$$log(ST) = 1.7 + 0.3\ log(DH)$$
$$log(Complexity) = -0.1 + 0.8\ log(DH)$$
$$log(H.A.C) = 0.5 + 0.2\ log(DH)$$
$$log(Density) = 6.7 - 1.1\ log(DH)$$
$$log(Index\ of\ Refraction) = 0.19 + 0.03\ log(DH).$$

6- Modified forgetten domination index

$$log(ST) = 2.001 + 0.3\ log(DF^*)$$
$$log(Complexity) = 0.4 + 0.8\ log(DF^*)$$
$$log(H.A.C) = 0.7 + 0.2\ log(DF^*)$$
$$log(Density) = 0.2 + 0.03\ log(DF^*)$$
$$log(Index\ of\ Refraction) = 0.2 + 0.03\ log(DF^*).$$

7- Domination Sombor index

$$log(ST) = 1.7 + 0.6\ log(DSO)$$
$$log(Complexity) = -0.22 + 1.4\ log(DSO)$$
$$log(H.A.C) = 0.5 + 0.4\ log(DSO)$$
$$log(Density) = 6.005 - 1.6\ log(DSO)$$
$$log(Index\ of\ Refraction) = 0.19 + 0.05\ log(DSO).$$

TABLE 3 The S.T and complexity values predicted by domination topological indices

Chemical Compound	S.T predicted by							Complexity predicted by						
	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO
1,4-Butanedithiol	35.3	48.07	35.8	32.87	27.06	29.7	35.66	81.1	69.78	63.5	15.3	64.2	61.2	63.63
2-Butanone	24.5	30.23	23.65	23.05	19.06	20.9	23.46	30.4	27.6	24.08	6.3	25.2	23.8	23.94
1,3-Butanediol	24.9	30.23	25.38	23.16	19.2	21.3	25.46	31.7	27.6	28.4	6.4	25.8	25.05	28.98
Butane dinitrile	35.4	48.07	35.85	32.87	27.06	24.7	35.66	81.1	69.78	63.56	15.3	64.2	61.28	63.63
Butanediamide	32.6	41.82	35.85	29.61	24.51	27.1	35.83	65.4	52.8	63.5	11.8	49.2	47.68	64.34
Butane-1-sulfonamide	39.7	56.09	44.57	35.85	30.42	33.5	44.38	110.4	95.01	105.6	19.07	87.6	83.89	106.01

1-Butanethiol	23.3	26.94	21.83	22.18	17.7	19.6	21.96	26.7	21.9	19.97	5.7	20.68	20.21	20.52
1,4-Diamonobutane	35.4	48.07	35.85	32.87	27.06	24.7	35.66	81.1	69.78	63.5	15.3	64.2	61.28	63.63
Butane-1,4-disulfonic acid	36.6	54.87	52.27	32.76	31.29	35.8	54.19	88.6	90.9	153.2	15.2	94.2	100.08	168.91
Butyraldehyde	23.3	26.9	21.83	22.18	17.7	19.65	21.96	26.7	21.9	19.9	5.7	20.68	20.21	20.52
2,3-Butanedione	25.9	33.05	27.04	23.9	20.38	22.36	26.82	35.2	33.002	32.9	6.9	30.1	28.53	32.74
1-Butanesulfonyl chloride	39.7	56.09	44.57	35.85	30.42	33.51	44.38	110.4	95.01	105.6	19.07	87.67	83.89	106.01

TABLE 4 The H.A.C and densitty values of predicted by domination topological indices.

Chemical Compound	H.A.C predicted by							Density predicted by						
	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO
1,4-Butanedithiol	5.719615	8.0008	5.733318	8.522983	4.78	5.0988152	5.75	1.89	2.39	2.8	2.2	2.3	2.2	2.73
1-Butanone	4.477865	5.65	4.345042	5.976146	3.78	4.027505	4.35	8.2	8.58	8.7	9.4	8.37	8.06	8.36
1,3-Butanediol	4.521774	5.65	4.554650	6.005732	3.8	4.076636	4.59	7.7	8.58	7.2	9.29	8.09	7.5	6.72
Butane dinitrile	5.719615	8.0008	5.733318	8.522983	4.78	5.0988152	5.75	1.89	2.39	2.8	2.2	2.3	2.2	2.73
Butanediamide	5.420829	7.2	5.733318	7.677765	4.47	4.788162	5.76	2.6	3.5	2.8	3.4	3.33	3.1	2.7
Butane-1-sulfonamide	6.173244	8.98	6.629017	9.294574	5.17	5.514553	6.65	1.189	1.56	1.6	1.6	1.5	1.4	1.52
1-Butanethiol	4.334658	5.18	4.119052	5.750585	3.6	3.863677	4.16	9.9	11.78	10.7	11.05	10.98	10.1	9.97
1,4-Diamonobutane	5.719615	8.0008	5.733318	8.522983	4.78	5.0988152	5.75	1.89	2.39	2.8	2.2	2.3	2.2	2.73
Butane-1,4-disulfonic acid	5.848275	8.83	7.372360	3.493393	5.27	5.763236	7.6	1.65	1.66	1.05	2.3	1.36	1.12	0.89
Butyraldehyde	4.334658	5.18	4.119052	5.750585	3.6	3.863677	4.16	9.9	11.78	10.7	11.05	10.98	10.1	9.97
2,3-Butanedione	4.644161	6.04	4.750704	6.198084	3.96	4.211319	4.75	6.59	6.7	6.09	8.19	6.55	6.3	5.85
1-Butanesulfonyl chloride	6.178244	8.98	6.629017	9294574	5.17	5.514553	6.65	1.18	1.56	1.6	1.6	1.5	1.4	1.52

TABLE 5 The refraction index values of predicted by domination topological indices.

Chemical Compound	Refraction index predicted by						
	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO
1,4-Butanedithiol	1.386226	1.429426	1.423739	1.36	1.418835	1.4	1.413663
1-Butanone	1.336256	1.364658	1.375242	1.31	1.369939	1.355	1.365177
1,3-Butanediol	1.338214	1.364658	1.383365	1.31	1.371205	1.357	1.374505
Butane dinitrile	1.386226	1.424426	1.423739	1.36	1.418835	1.4	1.413663
Butanediamide	1.375115	1.404649	1.423739	1.34	1.404830	1.39	1.414221
Butane-1-sulfonamide	1.402358	1.451648	1.449809	1.37	1.435497	1.42	1.439671
1-Butanethiol	1.329757	1.349044	1.366090	1.3	1.359831	1.34	1.357677
1,4-Diamonobutane	1.386226	1.429426	1.423739	1.36	1.418835	1.4	1.413663
Butane-1,4-disulfonic acid	1.39086	1.448469	1.469199	1.36	1.439555	1.43	1.463821
Butyraldehyde	1.329757	1.349044	1.366090	1.3	1.359831	1.34	1.35767
2,3-Butanedione	1.343585	1.376893	1.390671	1.31	1.379141	1.36	1.380506
1-Butanesulfonyl chloride	1.402358	1.451648	1.449809	1.37	1.435497	1.42	1.43967

The correlation coefficient values of predicted physiochemical properties of butane derivative with the exact values of this physico-chemical properties are given in Tables 6 (a), (b) and 7.

TABLE 6 :(a) The correlation coefficient values of predicted physicochemical properties with its exact values.

Physiochemical properties	S.T predicted by							Complexity predicted by						
	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO
S.T	0.57	0.63	0.804	0.53	0.67	0.712	0.83							
Complexity								0.6	0.7	0.89	0.53	0.734	0.8	0.904

(b)

Physiochemical properties	H.A.C predicted by							Density predicted by						
	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO
H.A.C	0.63	0.69	0.862	0.581	0.73	0.762	0.88							
Density								0.8	0.77	0.77	0.81	0.78	0.78	0.77

TABLE 7 The correlation coefficient values of predicted physicochemical properties with its exact values

Physiochemical properties	The refraction index predicted by						
	DM_1	DM_2	DM_1^*	DF	DH	DF^*	DSO
I.R	0.654	0.68	0.75	0.66	0.71	0.72	0.76

The following figures indicates how much the predicted values of physio-chemical properties are correlated with the well-known physio-chemical properties. The degree of correlation between any two data sets is measured by the correlation coefficent (R). During the R value becomes closed to unity, two datasets are more correlated. The QSPR study of domination topological indices reveals that these domination indices can be helpful in predicting Surface Tension (ST), complexity, Heavy Atomic Count (H.A.C), density, and refraction index. We can also note that the correlation coefficient values of the predicted values of Surface Tension (ST) and its exact values lies between the range of $0.53 \leq R \leq 0.83$ with the best correlation coefficient 0.83 of domination Sombor index (Figure 1). Furthermore, we can see the correlation coefficient values of the complexity predicted values with its exact values are lies between the range of $0.53 \leq R \leq 0.90$. Here, also the best value of correlation coefficient is 0.904 for domination Somber index (Figure 2). While based on Figure 3, the correlation range is $0.58 \leq R \leq 0.88$ which shows a good correlation of predicted values of (H.A.C) with exact values of (H.A.C). Figure 4 demonstrates that the correlation coefficient of density predicted values with its exact values are lies between the range of $0.77 \leq R \leq 0.81$. Finally, as Figure 5 indicates, the correlation range is $0.654 \leq R \leq 0.76$ which shows a good correlation coefficient of predicted values of refraction index with its exact values. In Figure 5, we can see that the correlation coefficient values of the domination Sombor index are the most highest. On the another hand, all domination indices are very useful to predict the physio-chemical properties of butane derivatives. Surface Tension (ST), complexity, Heavy Atomic Count (H.A.C), density and refraction index are important physico-chemical properties by using those domination indices to predict the values of these properties. It has been shown that these indices can beconsidered useful molecular descriptors in QSPR analysis of butane derivative.

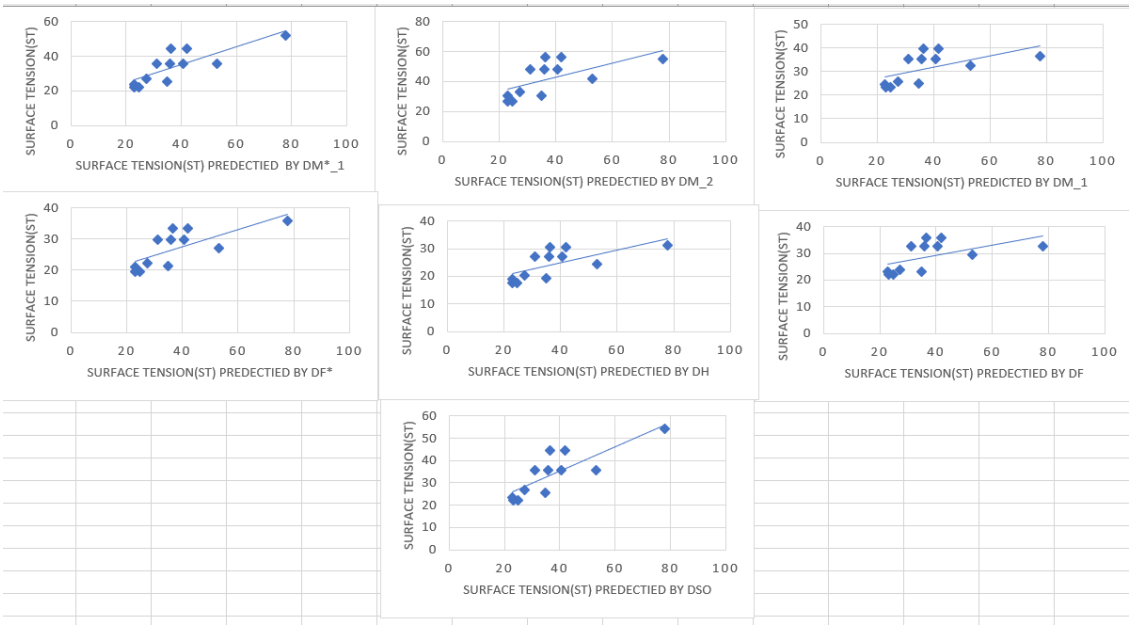

FIGURE 1 Graphical relationships between predicted values of Surface Tension (ST) and its exact values

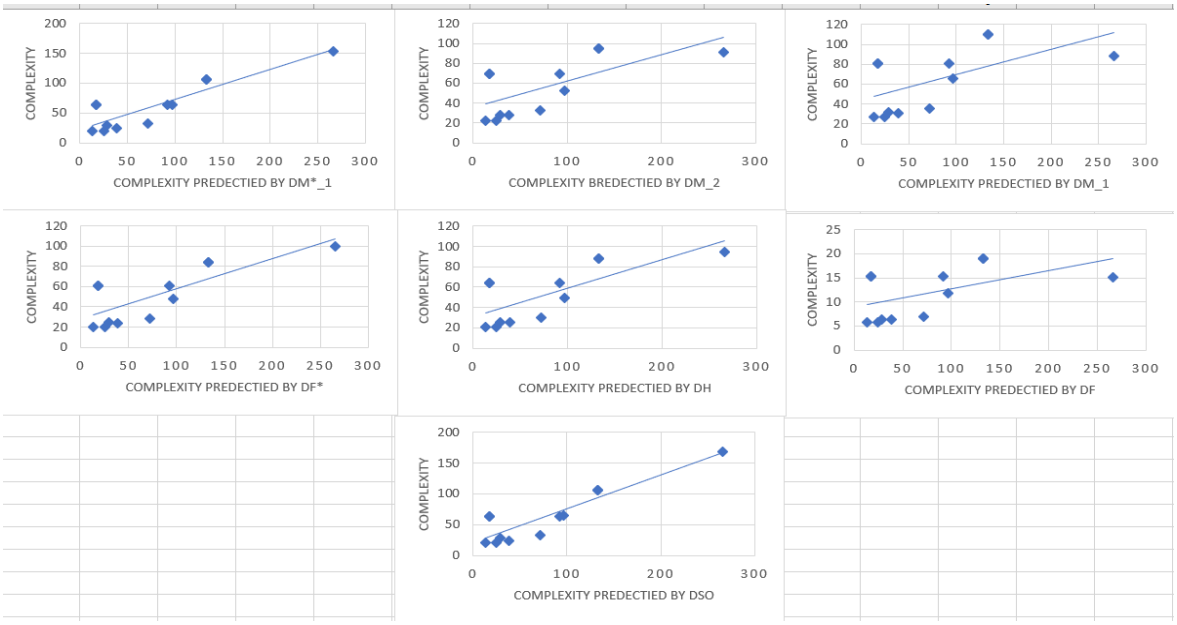

FIGURE 2 Graphical relationships between complexity predicted values and its exact values

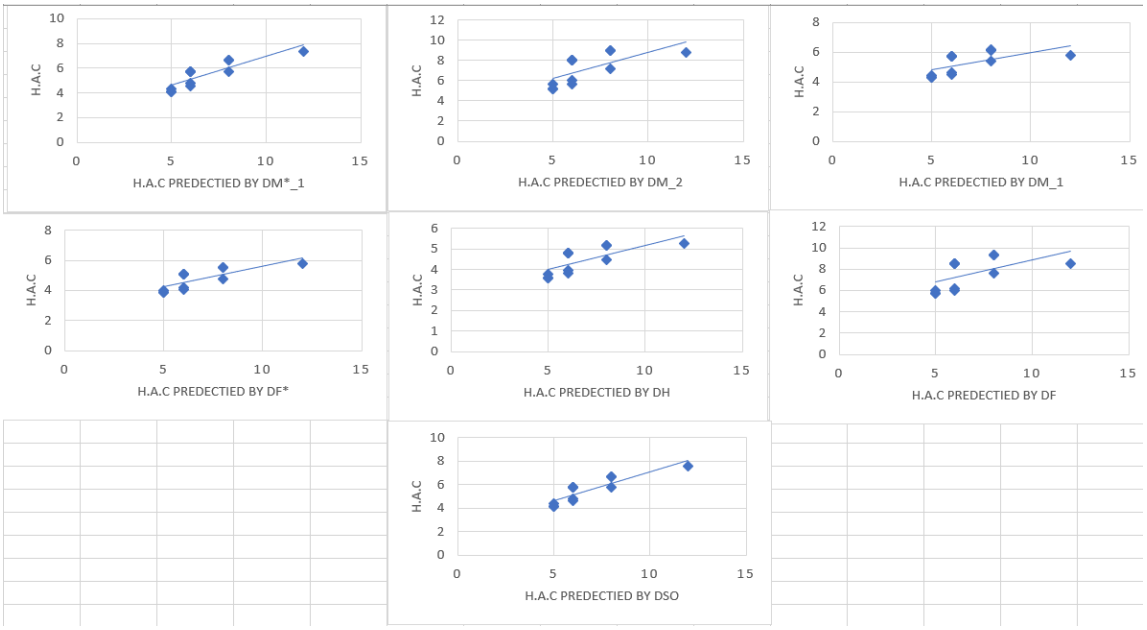

FIGURE 3 Graphical relationships between H.A.C predicted values and its exact values

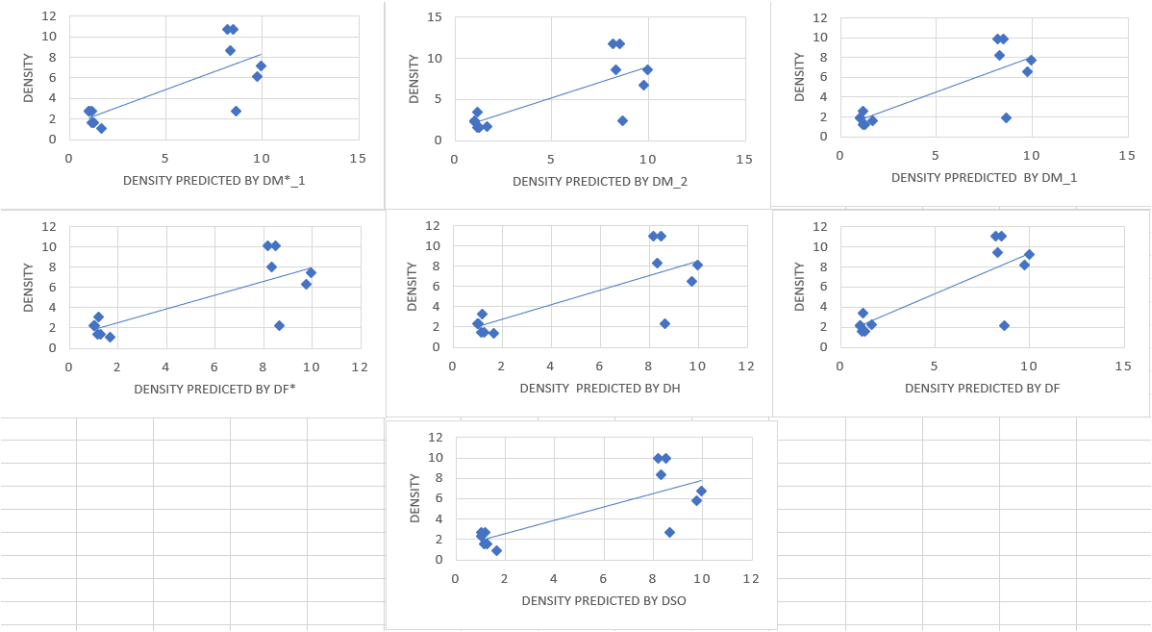

FIGURE 4 Graphical relationships between density predicted values and its exact values

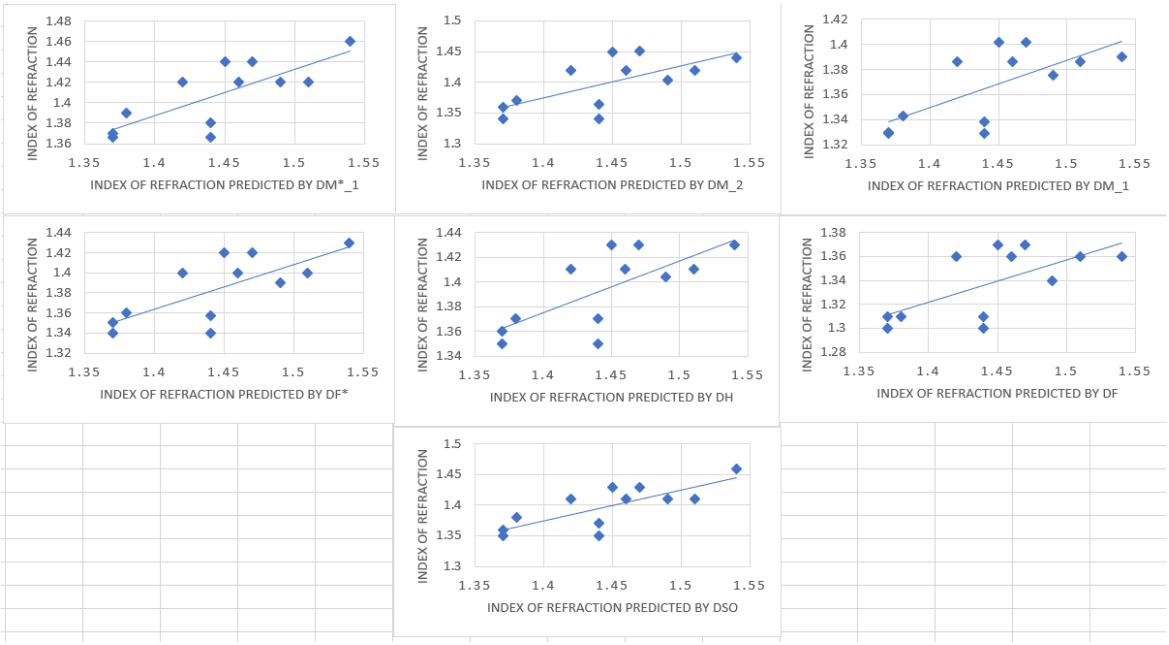

FIGURE 5 Graphical relationships between predicted values of refraction index and its values

Conclusion

In this research work, we defined a new topological index based on the minimal dominating sets. This index is the domination Sombor index. We calculated the exact values of the domination Sombor index of some families and some graph operations. Likewise, we defined the significance of the Sombor index in predicting the physicochemical properties of butane derivatives.

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Conflict of Interest

The authors declare that there is no conflict of Interest.

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