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On Sombor Indices of Some Structural Isomers

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Abstract
Some degree based topological indices can be used to predict chemical properties of molecular structures. Sombor index, reduced Sombor index and average Sombor index on chemical trees of some structural isomers are calculated. In particular Carbon structures of alcohol family with OH in 1st, 2nd, 3rd …. Positions are considered and derive Common formula to calculate the Sombor indices.

1. Introduction

Degree based topological indices have gained attention of researchers within a short span of time. Many such indices have been considered to find applications in Chemical graph theory. The Sombor index, the reduced Sombor index and the average Sombor index were introduced by the mathematician Ivan Gutman[2] who has significant contribution in chemical graph theory. More studies on Sombor index can be found in [3, 4, 6, 8, 9, 10,12]. Applicability of Sombor indices is examined in [5]. In this paper we consider chemical structures as finite, simple connected graphs. Structural isomers particularly from positional isomers structures with increased number of carbons of alcohol family are considered. Let G (V, E) be a graph with vertex set V(G) and edge set E(G) having p vertices and q edges respectively. The degree of a vertex u is the number of edges connected to u in G. It is denoted by d_u [1,11,4]. A connected acyclic graph is called a tree. The Sombor indices and their mathematical formulas are considered.

$SO(G)$, $SO_{red}(G)$, $SO_{avg}(G)$ are defined as [2]

$$SO(G) = \sum_{uv\in E(G)} \sqrt{{d_u}^2 + {d_v}^2}$$

$$SO_{red}(G) = \sum_{uv\in E(G)} \sqrt{(d_u - 1)^2 + (d_v - 1)^2}$$

$$SO_{avg}(G) = \sum_{uv\in E(G)} \sqrt{\left(d_u - \frac{2q}{p}\right)^2 + \left(d_v - \frac{2q}{p}\right)^2}$$

Tree structures of alcohol family with OH in different positions are categorized. Sombor indices of these categories are obtained for 100 structures of each category using C programming.

1. Method

The Sombor index, Reduced Sombor index and Average Sombor index for different tree categories are denoted by

(i) $SO(1-OH)=\sum_{uv\in E(1-OHT)}\sqrt{{d_u}^2+{d_v}^2}$

$$SO(2-OH)=\sum_{uv\in E(2-OHT)}\sqrt{{d_u}^2+{d_v}^2}$$

$$SO(3-OH)=\sum_{uv\in E(3-OHT)}\sqrt{{d_u}^2+{d_v}^2}$$

$SO(4-OH)=\sum_{uv\in E(4-OHT)}\sqrt{{d_u}^2+{d_v}^2}$ etc.

(ii) $SO_{red}(1-OH)=\sum_{uv\in E(1-OHT)}\sqrt{(d_u-1)^2+(d_v-1)^2}$

$$SO_{red}(2-OH)=\sum_{uv\in E(2-OHT)}\sqrt{(d_u-1)^2+(d_v-1)^2}$$

$$SO_{red}(3-OH)=\sum_{uv\in E(3-OHT)}\sqrt{(d_u-1)^2+(d_v-1)^2}$$

$$SO_{red}(4-OH)=\sum_{uv\in E(4-OHT)}\sqrt{(d_u-1)^2+(d_v-1)^2}$$

(iii) $SO_{avg}(1-OH)=\sum_{uv\in E(1-OHT)}\sqrt{\left(d_u-\frac{2q}{p}\right)^2+\left(d_v-\frac{2q}{p}\right)^2}$

$$SO_{avg}(2-OH)=\sum_{uv\in E(2-OHT)}\sqrt{\left(d_u-\frac{2q}{p}\right)^2+\left(d_v-\frac{2q}{p}\right)^2}$$

$$SO_{avg}(3-OH)=\sum_{uv\in E(3-OHT)}\sqrt{\left(d_u-\frac{2q}{p}\right)^2+\left(d_v-\frac{2q}{p}\right)^2}$$

$$SO_{avg}(4-OH)=\sum_{uv\in E(4-OHT)}\sqrt{\left(d_u-\frac{2q}{p}\right)^2+\left(d_v-\frac{2q}{p}\right)^2}$$

We obtained these indices for carbon chains with increasing carbons based on position of OH considered from positional isomers of alcohol family. Some alcohols of the different categories are presented in the following tables but we obtained Sombor indices for 100 carbon chains with OH in 1st position, OH attached to 2nd position, 3rd position and 4th position. Table 1 shows the Carbon chain with OH in first position. Table 2 shows the Carbon chain with OH attached to second position. Table 3 shows the Carbon chain with OH attached to third position. Table 4 shows the Carbon chain with OH attached to fourth position. Structural isomers particularly from positional isomers structures with increased number of carbons of alcohol family are considered number of carbons of alcohol family are considered.

Table 1 Carbon Chains with OH in First Position

Name	Nodes (p)	Edges(q)
Methanol	6	5
Ethanol	9	8
1-Propanol	12	11
1-Butanol	15	14
1-Pentanol	18	17
1-Hexanol	21	20
1-Heptanol	24	23
1-Octanol	27	26

Table 2 Carbon Chains with OH Attached to Second Position

Structure Name	Nodes (n)	Edges(m)
2-proponal	12	11
2-Butanol	15	14
2-Pentanol	18	17
2-Hexanol	21	20
2-Heptanol	24	23
2-Octanol	27	26

Table 3 Carbon Chains with OH Attached to Third Position

Structure Name	Nodes (n)	Edges(m)
3-Pentanol	18	17
3-Hexonol	21	20
3-Heptanol	24	23
3-Octanol	27	26

Table 4 Carbon Chains with OH Attached to Fourth Position

Structure Name	Nodes(n)	Edges(m)
4-Heptanol	24	23
4-Octanol	27	26
4-Nonanol	30	29
4-Decanol	33	32

2. Results and Discussions

2.1 Proposition 1

Let G be a tree T with $p \geq 6$ vertices, $q \geq 5$ edges with $(2n+1)$ edges having vertex degrees $d_{u_1} = 1, d_{v_1} = 4$, (n – 1) edges having vertex degrees $d_{u_2} = 4, d_{v_2} = 4$, one edge having vertex degrees $d_{u_3} = 2, d_{v_3} = 4$, one edge having vertex degrees $d_{u_4} = 1, d_{v_4} = 2$ where n = 1, 2, 3, 4, ……. The Sombor index is,

$$SO(1-OH) = (2n+1)\sqrt{17} + (n-1)4\sqrt{2} + 3\sqrt{5}, \quad n = 1, 2, 3, 4, \ldots.$$

Proof: Consider Methanol structure as tree T with $p = 6$ vertices and $q = 5$ edges. Figure 1 shows the Methanol

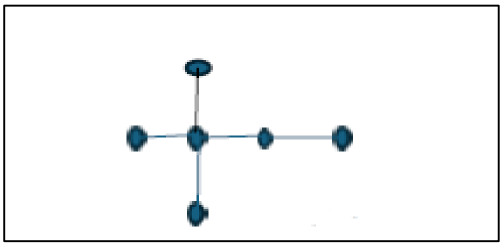

Figure 1 Methanol

The Sombor index is

$$SO(Methanol) = (2n+1)\sqrt{17} + (n-1)4\sqrt{2} + 3\sqrt{5}, for\ n = 1$$

Tree for Ethanol structure is obtained by adding 3 vertices and 3 edges to figure 1. Figure 2 shows the Ethanol

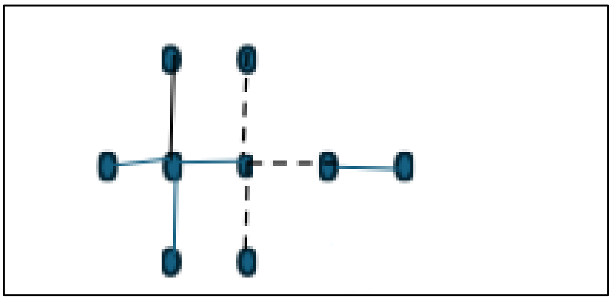

Figure 2 Ethanol

The Sombor index is

$$SO(Ethanol) = (2n+1)\sqrt{17} + (n-1)4\sqrt{2} + 3\sqrt{5}, for\ n = 2.$$

Adding 3 vertices and 3 edges to figure 2 gives 1-Propanol. Figure 3 shows the Propanol.

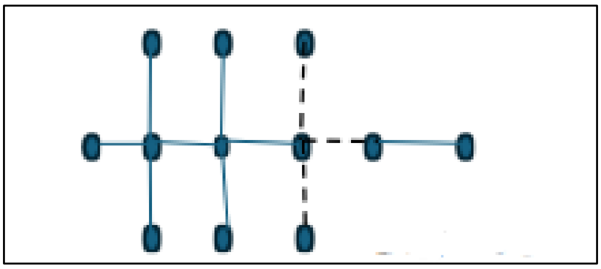

Figure 3 Propanol

The Sombor index is

SO(1-Propanol) =(2n+1) √17+(n-1)4√2+3√5, for n=3.

Continuation of attaching 3 vertices and 3 edges to immediate preceding trees gives chemical trees of 1-Butanol, 1-Pentanol, 1-Hexanol, 1-Heptanol, …. structures. The Sombor indices of these are obtained by (2n+1) √17+(n-1)4√2+3√5 ,for n=4,5,6,7,…. respectively. The Sombor index of all Carbon chains of alcohol family with OH in first position can be obtained by

SO(1-OH)=(2n+1) √17+(n-1)4√2+3√5 ,n=1,2,3,4,….

2.2 Proposition

Let G be a tree T with p≥6 vertices, q≥5 edges with (2n+1) edges having vertex degrees d_(u_1)=1,d_(v_1)=4, (n – 1) edges having vertex degrees d_(u_2)=4,d_(v_2)=4 , one edge having vertex degrees d_(u_3)=2,d_(v_3)=4, one edge having vertex degrees

d_(u_4)=1,d_(v_4)=2 where n = 1, 2, 3, 4,…

The reduced Sombor index is

〖SO〗_red (1-OH)=(2n+1)3+(n1)3√2+√10+1,n=1,2,3,4,….

Proof: Methanol structure is considered as tree T with p=6 vertices and q=5 edges.

The reduced Sombor index is obtained by

〖SO〗_red (Methanol)=(2n+1)3+(n-1)3√2+√10+1, for n=1

Including 3 vertices and 3 edges to Methanol tree gives Ethanol tree as depicted in figure 2.

The reduced Sombor index of Ethanol tree is

〖SO〗_red (Ethanol)=(2n+1)3+(n-1)3√2+√10+1, for n=2

Chemical Tree of 1-Propanol as constructed in figure 3 by attaching 3 vertices and three edges to Ethanol tree has reduced Sombor index,

〖SO〗_red (1-Proponal) =(2n+1)3+(n-1)3√2+√10+1, for n=3.

The reduced Sombor index of all Carbon chains of alcohol family with OH in first position can be obtained by

〖SO〗_red (1-OH) =(2n+1)3+(n1)3√2+√10+1, n=1,2,3,4,5……

2.3 Proposition 3

Let G be a tree T with p≥6 vertices, q≥5 edges with (2n+1) edges having vertex degrees d_ (u_1) =1,d_(v_1)=4, (n – 1) edges having vertex degrees d_(u_2)=4,d_(v_2)=4 , one edge having vertex degrees d_(u_3)=2,d_(v_3)=4, one edge having vertex degrees

d_ (u_4) =1, d_ (v_4) =2 where n = 1, 2, 3, 4, …….

The average Sombor index is

$$\text{SO〗avg(1-OH)}=(2n+1)\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+(n-1)\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]\sqrt{2}$$

$$+\sqrt{\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2},n=1,2,3,4,5,\ldots\ldots$$

Proof: The tree of Methanol structure has $p=3n+3, n=1$ vertices and $q=3n+2, n=1$ edges. The average Sombor index is obtained by

$SO_{avg}(Methanol)$

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

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

$for\ n=1$, when 3 vertices and 3 edges are added to Methanol tree gives Ethanol tree with $p=3n+3, n=2$ vertices and $q=3n+2, n=2$ edges as depicted in figure 2.The average Sombor index of Ethanol tree is

$$SO_{avg}(Ethanol) = (2n+1)\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+(n-1)\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]\sqrt{2}$$

$$+\sqrt{\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}$$

$for\ n=2$

Chemical Tree of 1-Propanol with $p=3n+3, n=3$ vertices and $q=3n+2, n=3$ edges as constructed in figure 3 by attaching 3 vertices and three edges to Ethanol tree has average Sombor index ,

$$SO_{avg}(1-Proponal) = (2n+1)\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+(n-1)\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]\sqrt{2}$$

$$+\sqrt{\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}$$

$$for\ n=3$$

The average Sombor index of all Carbon chains of alcohol family with OH in first position can be obtained by Chemical Tree of 1-Propanol as constructed in figure 3 by attaching 3 vertices and three edges to Ethanol tree has reduced Sombor index,

$$SO_{avg}(1-OH) = (2n+1)\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+(n-1)\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]\sqrt{2}+$$

$$\sqrt{\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}\quad n=1,2,3,4,5\ ....$$

Observation 1: For all alcohol structures when OH is attached to second carbon gives 2-Proponal, 2-Butanol, 2-Pentanol, 2-Hexanol, The Sombor indices of these structures are obtained by

$$SO(2-OH) = (2n+1)\sqrt{17}+(n-1)4\sqrt{2}+3\sqrt{5}\,,\qquad n=\ 3,4,5,....$$

$$SO_{red}(2-OH) = (2n+1)3+(n-1)3\sqrt{2}+\sqrt{10}+1\,,\ \ n=\ 3,4,5,\dots....$$

$$SO_{avg}(2-OH) = (2n+1)\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+\ (n-1)\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]\sqrt{2+}$$

$$\sqrt{\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2} \qquad n = 3,4,5,....$$

Observation 2: For all alcohol structures when OH is attached to third carbon gives 3-Pentanol, 3-Hexanol, The Sombor indices of these structures are obtained by

$$SO(3-OH) = (2n+1)\sqrt{17}+(n-1)4\sqrt{2}+3\sqrt{5}, \qquad n = 5,6,7,....$$

$$SO_{red}(3-OH) = (2n+1)3+(n-1)3\sqrt{2}+\sqrt{10}+1, \quad n = 5,6,7,.......$$

$$SO_{avg}(3-OH) = (2n+1)\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+(n-1)\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]\sqrt{2}+$$
$$\sqrt{\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2} \qquad n = 5,6,7,...$$

Observation 3: For all alcohol structures when OH is attached to fourth carbon gives 4-Heptanol, 4-Nonanol, 4-Deconal ……. The Sombor indices of these structures are obtained by

$$SO(4-OH) = (2n+1)\sqrt{17}+(n-1)4\sqrt{2}+3\sqrt{5}, \qquad n = 7,8,9,....$$

$$SO_{red}(4-OH) = (2n+1)3+(n-1)3\sqrt{2}+\sqrt{10}+1, \quad n = 7,8,9,.......$$

$$SO_{avg}(4-OH) = (2n+1)\sqrt{\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+(n-1)\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]\sqrt{2}+$$

$$\sqrt{\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[4-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2}+\left[1-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2+\left[2-\left(\frac{2(3n+2)}{3n+3}\right)\right]^2 \qquad n = 7,8,9,.......$$

Following Table 1 values of Sombor indices are obtained using C programing

Table 5 Sombor Indices of Alcohol Carbon Chains with OH in First Position

$SO(1-OH)$	$SO_{red}(1-OH)$	$SO_{avg}(1-OH)$
19.07752	13.16228	10.38249
32.98059	23.40492	17.95691
46.88365	33.64756	25.40095
60.78672	43.89020	32.78923
74.68978	54.13284	40.14884
88.59285	64.37548	47.49185
102.49591	74.61812	54.82437
116.39898	84.86076	62.14986
130.30204	95.10340	69.47041
144.20511	105.34604	76.78735
158.10818	115.58868	84.10158
172.01124	125.83133	91.41372
185.91431	136.07397	98.72422
199.81737	146.31661	106.03340
213.72044	156.55925	113.34151
227.62350	166.80189	120.64873
241.52657	177.04453	127.95522
255.42963	187.28717	135.26108
269.33270	197.52981	142.56642
283.23577	207.77245	149.87130
297.13883	218.01509	157.17579
311.04190	228.25773	164.47994
324.94496	238.50037	171.78380
338.84803	248.74301	179.08739
352.75109	258.98565	186.39075
366.65416	269.22829	193.69390
380.55722	279.47094	200.99687
394.46029	289.71358	208.29967
408.36335	299.95622	215.60232
422.26642	310.19886	222.90484
436.16949	320.44150	230.20724

450.07255	330.68414	237.50952
463.97562	340.92678	244.81171
477.87868	351.16942	252.11380
491.78175	361.41206	259.41581
505.68481	371.65470	266.71774
519.58788	381.89734	274.01959
533.49094	392.13998	281.32138
547.39401	402.38262	288.62311
561.29708	412.62526	295.92479
575.20014	422.86791	303.22641
589.10321	433.11055	310.52798
603.00627	443.35319	317.82950
616.90934	453.59583	325.13099
630.81240	463.83847	332.43243
644.71547	474.08111	339.73384
658.61853	484.32375	347.03521
672.52160	494.56639	354.33654
686.42466	504.80903	361.63785
700.32773	515.05167	368.93913
714.23080	525.29431	376.24038
728.13386	535.53695	383.54160
742.03693	545.77959	390.84280
755.93999	556.02223	398.14398
769.84306	566.26487	405.44513
783.74612	576.50752	412.74627
797.64919	586.75016	420.04738
811.55225	596.99280	427.34848
825.45532	607.23544	434.64955
839.35839	617.47808	441.95061
853.26145	627.72072	449.25166
867.16452	637.96336	456.55269
881.06758	648.20600	463.85370
894.97065	658.44864	471.15471
908.87371	668.69128	478.45569
922.77678	678.93392	485.75667
936.67984	689.17656	493.05763
950.58291	699.41920	500.35858
964.48597	709.66184	507.65952
978.38904	719.90449	514.96045
992.29211	730.14713	522.26137
1006.19517	740.38977	529.56228
1020.09824	750.63241	536.86318
1034.00130	760.87505	544.16408
1047.90437	771.11769	551.46496
1061.80743	781.36033	558.76583
1075.71050	791.60297	566.06670
1089.61356	801.84561	573.36756
1103.51663	812.08825	580.66841
1117.41970	822.33089	587.96925
1131.32276	832.57353	595.27009
1145.22583	842.81617	602.57092
1159.12889	853.05881	609.87175
1173.03196	863.30145	617.17257
1186.93502	873.54410	624.47338
1200.83809	883.78674	631.77419
1214.74115	894.02938	639.07499
1228.64422	904.27202	646.37578
1242.54728	914.51466	653.67657
1256.45035	924.75730	660.97736
1270.35342	934.99994	668.27814
1284.25648	945.24258	675.57892
1298.15955	955.48522	682.87969
1312.06261	965.72786	690.18046
1325.96568	975.97050	697.48122
1339.86874	986.21314	704.78198
1353.77181	996.45578	712.08273
1367.67487	1006.69842	719.38348
1381.57794	1016.94106	726.68423
1395.48101	1027.18371	733.98497

Same values of above three Sombor indices are observed for 2 – OH, 3 – OH, 4 – OH categories beginning from 3^{rd}, 5^{th}, 7^{th} values respectively.

Conclusion

In this paper categories of alcohol family structures based on OH molecules position are used to derive common formulae and to calculate Sombor indices using C programing. These results may be useful in developing models to examine chemical applicability of the Sombor indices.

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