

Diagrammatic representation between Topological indices and Alkanes

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Received: 2022 March 15; **Revised:** 2022 April 20; **Accepted:** 2022 May 10.

Abstract

In this article we have to study the diagrammatic representation between Topological indices and Alkanes. Most of the researchers have done a wonderful result in their research activities in the similar field. But here, we can see the diagrammatic representation between Topological indices and 67 Alkanes. In this article, I am taking three types of topological indices namely Wiener index, Hyper Wiener index and Terminal Wiener index of 67 Alkanes. I also take Range chart of 67 alkanes and the three types of Wiener indices. Range chart is a very good method of showing the range of variation that is the minimum and the maximum values of a variable. For example if we are interested in showing the difference between the physico-chemical properties of 67 alkanes and the three types of Wiener indices.

Keywords: Range chart, Wiener index, Alkanes, Terminal Wiener index and Hyper Wiener index

Introduction

Graph theory is ultimately the study of relationships. Given a set of nodes and

connections, which can abstract anything from city layouts to computer data, graph theory provides a helpful tool to quantify

and simplify the many moving parts of dynamic systems. Studying graphs through a framework provides answers to many arrangement, networking optimization, matching and operational problems. Transforming a chemical structure into a number actually is called a topological index. It means a graph that is remains invariant under graph automorphism and a graph which is characterized always invariant. It plays a vital role in chemical graph theory. A topological graph is otherwise called molecular descriptor and that can be use in any graph which models some molecular structure and we say that is a mathematical formula. Hence this efficient

method is to avoid expensive and to consume in laboratory experiments. Mathematical chemistry, especially in quantitative structure property relationship (QSPR) and quantitative activity relationship (QSAR) investigations play the most important role in molecular descriptors. In this article we are taking the three types of Wiener indices (Wiener index, Terminal Wiener index, Hyper Wiener index) and the five physico-chemical properties of 67 alkanes. Also we are taking the Range chart between the three types of topological indices and the five physico chemical properties of 67 alkanes.

Table 1

The table 1 shows the 67 alkanes and its Five physico chemical properties

S.No.	Alkane	bp(°C)	mv(cm ³)	mr(cm ³)	hv(kJ)	ct(°C)
1	Butane	-0.500				152.01
2	2-methylpropane	-11.730				134.98
3	Pentane	36.074	115.205	25.2656	26.42	196.62
4	2-methylbutane	27.852	116.426	25.2923	24.59	187.70
5	2,2dimethylpropane	9.503	112.074	25.7243	21.78	160.60
6	Hexane	68.740	130.688	29.9066	31.55	234.70

7	2-methylpentane	60.271	131.933	29.9459	29.86	224.90
8	3-methylpentane	63.282	129.717	29.8016	30.27	231.20
9	2,2-methylbutane	49.741	132.744	29.9347	27.69	216.20
10	2,3-dimethylbutane	57.988	130.240	29.8104	29.12	227.10
11	Heptanes	98.427	146.540	34.5504	36.55	267.55
12	2-methylhexane	90.052	147.656	34.5908	34.80	257.90
13	3-methylhexane	91.850	145.821	34.4597	35.08	262.40
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60
15	2,2-dimethylpentane	79.197	148.695	34.6166	32.43	247.70
16	2,3-dimethylpentane	89.784	144.153	34.3237	34.24	264.60
17	2,4-dimethylpentane	80.500	148.949	34.6192	32.88	247.10
18	3,3-dimethylpentane	86.064	144.530	34.3323	33.02	263.00
19	Octane	125.665	162.592	39.1922	41.48	296.20
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00
21	3-methylheptane	118.925	161.832	39.1001	39.83	292.00
22	4-methylheptane	117.709	162.105	39.1174	39.67	290.00
23	3-ethylhexane	118.53	160.07	38.94	39.40	292.00
24	2,2-dimethylhexane	10.84	164.28	39.25	37.29	279.00
25	2,3-dimethylhexane	115.607	160.39	38.98	38.79	293.00
26	2,4-dimethylhexane	109.42	163.09	39.13	37.76	282.00
27	2,5-dimethylhexane	109.10	164.69	39.25	37.86	279.00
28	3,3-dimethylhexane	111.96	160.87	39.00	37.93	290.84
29	3,4-dimethylhexane	117.72	158.81	38.84	39.02	298.00
30	3-ethyl-2-methylpentane	115.65	158.79	38.83	38.52	295.00

31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00
33	2,2,4-trimethylpentane	99.23	165.08	39.26	35.13	271.15
34	2,3,3-trimethylpentane	114.76	157.29	38.76	37.22	303.00
35	2,3,4-trimethylpentane	113.46	158.85	38.86	37.61	295.00
36	Nonane	150.79	178.71	43.84	46.44	322.00
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00
41	4-ethylheptane	141.20	175.68	43.49	44.81	318.30
42	2,2-dimethylheptane	132.69	180.50	43.91	42.28	302.00
43	2,3-dimethylheptane	140.50	176.65	43.63	43.79	315.00
44	2,4-dimethylheptane	133.50	179.12	43.73	42.87	306.00
45	2,5-dimethylheptane	136.00	179.37	43.84	43.87	307.80
46	2,6-dimethylheptane	135.21	180.91	43.92	42.82	306.00
47	3,3-dimethylheptane	137.300	176.897	43.6870	42.66	314.00
48	3,4-dimethylheptane	140.600	175.349	43.5473	43.84	322.70
49	3,5-dimethylheptane	136.000	177.386	43.6379	42.98	312.30
50	4,4-dimethylheptane	135.200	176.897	43.6022	42.66	317.80

51	3-ethyl-2-methylhexane	138.000	175.445	43.6550	43.84	322.70
52	4-ethyl-2-methylhexane	133.800	177.386	43.6472	42.98	330.30
53	3-ethyl-3-methylhexane	140.600	173.077	43.2680	44.04	327.20
54	2,2,4-trimethylhexane	126.540	179.220	43.7638	40.57	301.00
55	2,2,5-trimethylhexane	124.084	181.346	43.9356	40.17	296.60
56	2,3,3-trimethylhexane	137.680	173.780	43.4347	42.23	326.10
57	2,3,4-trimethylhexane	139.000	173.498	43.4917	42.93	324.20
58	2,3,5-trimethylhexane	131.340	177.656	43.6474	41.42	309.40
59	3,3,4-trimethylhexane	140.460	172.055	43.3407	42.28	330.60
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60
62	2,3-dimethyl-3-ethylpentane	142.000	170.093	42.9542	42.55	338.60
63	2,4-dimethyl-3-ethylpentane	136.730	173.804	43.4037	42.93	324.20
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50
65	2,2,3,4-tetramethylpentane	133.016	173.557	43.4359	41.00	319.60
66	2,2,4,4-tetramethylpentane	122.284	178.256	43.8747	38.10	301.60
67	2,3,3,4-tetramethylpentane	141.551	169.928	43.2016	41.75	334.50

Table 2 The table 2 shows that the calculation value between 67 alkanes and the three types of Wiener indices.

S.No.	Alkane	$W(G)$	$TW(G)$	$HW(G)$
1	Butane	10	3	46
2	2-methylpropane	9	6	27
3	Pentane	20	8	146
4	2-methylbutane	18	8	90
5	2,2dimethylpropane	16	8	52
6	Hexane	35	5	371
7	2-methylpentane	32	10	254
8	3-methylpentane	31	10	217
9	2,2-methylbutane	26	15	142
10	2,3-dimethylbutane	29	16	161
11	Heptanes	56	6	812
12	2-methylhexane	52	12	604
13	3-methylhexane	50	12	506
14	3-ethylpentane	48	12	408
15	2,2-dimethylpentane	49	16	370
16	2,3-dimethylpentane	46	15	352
17	2,4-dimethylpentane	48	16	426
18	3,3-dimethylpentane	44	14	296
19	Octane	84	7	1596
20	2-methylheptane	79	14	1261
21	3-methylheptane	76	14	1072
22	4-methylheptane	75	14	1011
23	3-ethylhexane	72	14	822
24	2,2-dimethylhexane	71	21	845

25	2,3-dimethylhexane	71	22	766
26	2,4-dimethylhexane	71	23	803
27	2,5-dimethylhexane	74	24	962
28	3,3-dimethylhexane	67	21	649
29	3,4-dimethylhexane	68	22	668
30	3-ethyl-2-methylpentane	67	22	607
31	3-ethyl-3-methylpentane	64	21	514
32	2,2,3-trimethylpentane	63	27	495
33	2,2,4-trimethylpentane	66	32	606
34	2,3,3-trimethylpentane	60	27	458
35	2,3,4-trimethylpentane	65	32	551
36	Nonane	120	8	2892
37	2-methyloctane	114	16	2388
38	3-methyloctane	110	16	2076
39	4-methyloctane	108	16	1920
40	3-ethylheptane	105	16	1604
41	4-ethylheptane	102	16	1452
42	2,2-dimethylheptane	104	24	1718
43	2,3-dimethylheptane	102	25	1548
44	2,4-dimethylheptane	102	26	1524
45	2,5-dimethylheptane	110	27	1646
46	2,6-dimethylheptane	108	28	1926
47	3,3-dimethylheptane	98	24	1340
48	3,4-dimethylheptane	98	25	1298
49	3,5-dimethylheptane	100	26	1396
50	4,4-dimethylheptane	96	24	1218
51	3-ethyl-2-methylhexane	96	25	1146

52	4-ethyl-2-methylhexane	98	26	1244
53	3-ethyl-3-methylhexane	92	24	992
54	2,2,4-trimethylhexane	94	36	1108
55	2,2,5-trimethylhexane	98	38	1328
56	2,3,3-trimethylhexane	90	32	936
57	2,3,4-trimethylhexane	92	36	992
58	2,3,5-trimethylhexane	96	38	1188
59	3,3,4-trimethylhexane	87	34	838
60	3,3-diethylpentane	88	24	796
61	2,2-dimethyl-3-ethylpentane	88	32	814
62	2,3-dimethyl-3-ethylpentane	86	34	740
63	2,4-dimethyl-3-ethylpentane	90	36	870
64	2,2,3,3-tetramethylpentane	82	44	628
65	2,2,3,4-tetramethylpentane	86	47	758
66	2,2,4,4-tetramethylpentane	86	40	850
67	2,3,3,4-tetramethylpentane	84	47	729

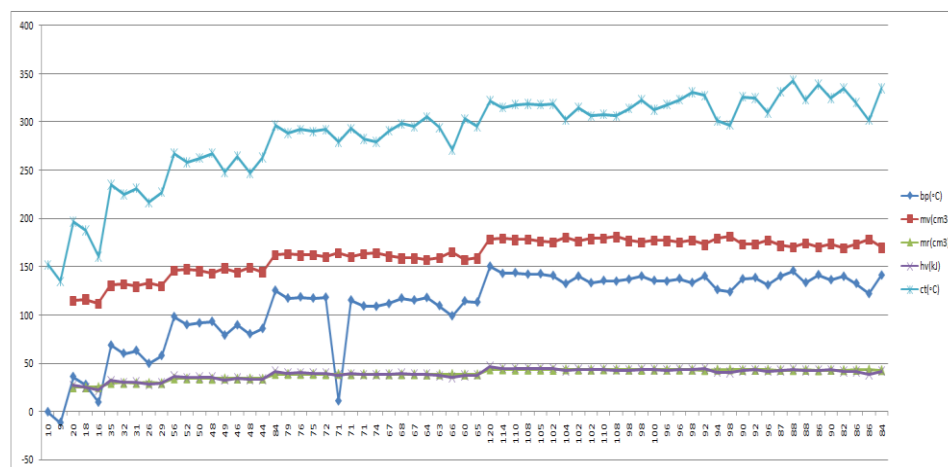
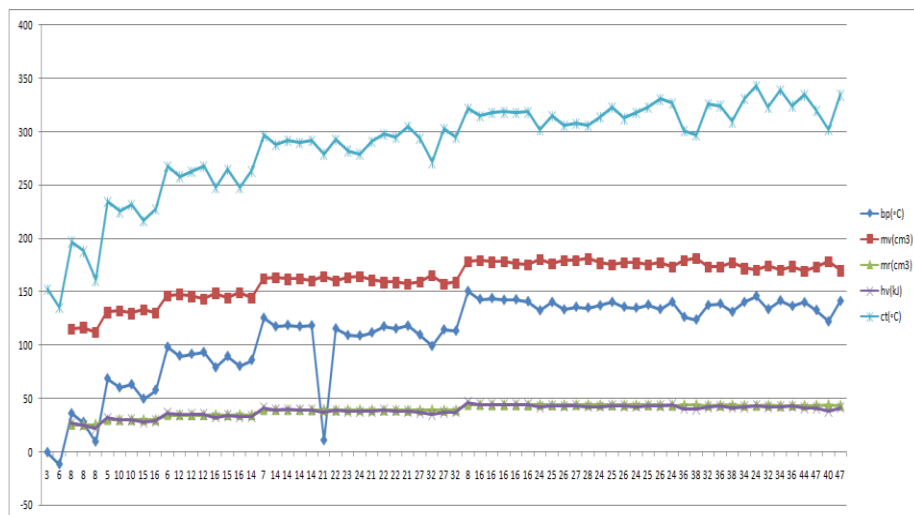
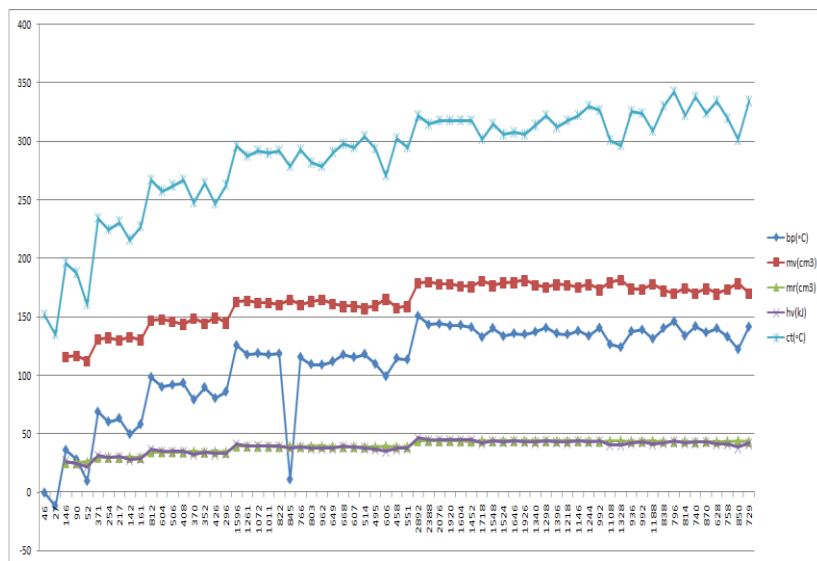
Figure 1: Range chart of $W(G)$ 

Figure 2: Range chart of TW(G)**Figure 3: Range chart of HW(G)**

Conclusion

In this article, I am taking three types of topological indices namely Wiener index,

Hyper Wiener index and Terminal Wiener index of 67 Alkanes .In this article we have seen that the Range chart of the three

topological indices (Wiener indices, Hyper Wiener indices and Terminal Wiener indices) and the Five physico-chemical properties of 67 alkanes.

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