

Applications of Domination Parameters in QSPR Studies

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Received: 10 February 2021/ Accepted: 08 March 2022/ Published online: 04 April 2022

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Abstract

A subset $D \subseteq V$ is a dominating set of a graph $G = (V, E)$ if $N[D] = V$. In this paper, we explore the applications of certain domination parameters in QSPR-studies.

Key words: Domination number, connected domination number, independent domination number, total domination number, QSPR-analysis.

AMS classification:05C90; 05C35; 05C69.

Introduction

A set D of vertices in a graph G is a dominating set if every vertex in $V - D$ is adjacent to some vertex in D . The **domination number** $\gamma(G)$ of G is the minimum cardinality of a dominating set of G [2]. A minimum dominating set of a graph G is called a γ -set of G .

- A dominating set D is a connected dominating set if $\langle D \rangle$ is connected [9].
- A dominating set D is independent dominating set if $\langle D \rangle$ is independent [1].
- A dominating set D is called a total dominating set if there are no isolates in $\langle D \rangle$ [3].
- A dominating set D is called a split dominating set if $\langle V - D \rangle$ is disconnected [7].
- A dominating set D is called a non-split dominating set if $\langle V - D \rangle$ is connected [8].

The minimum cardinality taken over all connected \ independent \ total \ split \ nonsplit \ cototal gives the respective domination numbers $\gamma_c(G)$ \ $\gamma_i(G)$ \ $\gamma_t(G)$ \ $\gamma_s(G)$ \ $\gamma_{ns}(G)$. For more details on domination parameters can be found in [4–6].

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The Use of Selected Domination Parameters in QSPR Studies

We have used here 06 domination parameters, viz., domination number $\gamma(G)$, connected domination number $\gamma_c(G)$, independent domination number $\gamma_i(G)$, total domination number $\gamma(t)(G)$, split domination number $\gamma_s(G)$ and non-split domination number $\gamma_{ns}(G)$ for modeling eight representative physical properties [boiling points(BP), molar volumes (mv) at 20°C, molar refractions (mr) at 20°C, heats of vaporization (hv) at 25°C, surface tensions (st) 20°C and melting points (mp)] of the 67 alkanes from n-butanes to nonanes. Values for these property were taken from [10]. The above said distance-based topological indices and the experimental values for the physical properties of 67 alkanes are listed in Table 1.

Table 1. Physical Properties of alkanes.



Table 1.

S.No.	Alkane	bp(°C)	mv(cm ³)	nr(cm ³)	lv(kJ)	et(°C)	ep(atm)	st(dyne/cm)	mp(°C)
1	Butane	-0.500				152.01	37.47		-138.35
2	2-methyl propane	-11.730				134.98	36		-150.60
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00	-129.72
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.70	32.9	15.00	-159.90
5	2,2 dimethylpropane	9.503	112.074	25.7243	21.78	160.60	31.57		-16.55
6	Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42	-95.35
7	2-methylpentane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38	-153.67
8	3-methylpentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12	-118.00
9	2,2-methylbutane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30	-99.87
10	2,3-dimethylbutane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37	-128.54
11	Heptanes	98.427	146.540	34.5504	36.55	267.55	27.01	20.26	-90.61
12	2-methylhexane	90.052	147.656	34.5008	34.80	257.90	27.2	19.29	-118.28
13	3-methylhexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79	-119.40
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44	-118.60
15	2,2-dimethylpentane	79.197	148.695	34.6166	32.43	247.70	28.4	18.02	-123.81
16	2,3-dimethylpentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96	-119.10
17	2,4-dimethylpentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15	-119.24
18	3,3-dimethylpentane	86.064	144.530	34.3323	33.02	263.00	30	19.59	-134.46
19	Octane	125.665	162.592	39.1922	41.48	296.20	24.64	21.76	-56.79
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60	-109.04
21	3-methylheptane	118.925	161.832	39.1001	39.83	292.00	25.6	21.17	-120.50
22	4-methylheptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00	-120.95

S.No.	Alkane	bp(°C)	mv(cm ³)	mr(cm ³)	lv(kJ)	ct(°C)	cp(atm)	st(dyne/cm)	mp(°C)
23	3-ethylhexane	118.53	160.07	38.94	39.40	292.00	25.74	21.51	
24	2,2-dimethylhexane	10.84	164.28	39.25	37.29	279.00	25.6	19.60	-121.18
25	2,3-dimethylhexane	115.007	160.39	38.98	38.79	293.00	26.6	20.99	
26	2,4-dimethylhexane	109.42	163.09	39.13	37.76	282.00	25.8	20.05	-137.50
27	2,5-dimethylhexane	109.10	164.69	39.25	37.86	279.00	25	19.73	-91.20
28	3,3-dimethylhexane	111.96	160.87	39.00	37.93	290.84	27.2	20.63	-126.10
29	3,4-dimethylhexane	117.72	158.81	38.84	39.02	298.00	27.4	21.64	
30	3-ethyl-2-methylpentane	115.65	158.79	38.83	38.52	295.00	27.4	21.52	-114.96
31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99	-90.87
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67	-112.27
33	2,2,4-trimethylpentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77	-107.38
34	2,3,3-trimethylpentane	114.76	157.29	38.76	37.22	303.00	29	21.56	-100.70
35	2,3,4-trimethylpentane	113.46	158.85	38.86	37.61	295.00	27.6	21.14	-109.21
36	Nonane	150.79	178.71	43.84	46.44	322.00	22.74	22.92	-53.52
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00	23.6	21.88	-80.40
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00	23.7	22.34	-107.64
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30	23.06	22.34	-113.20
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81	-114.90
41	4-ethylheptane	141.20	175.68	43.49	44.81	318.30	23.98	22.81	
42	2,2-dimethylheptane	132.69	180.50	43.91	42.28	302.00	22.8	20.80	-113.00
43	2,3-dimethylheptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34	-116.00
44	2,4-dimethylheptane	133.50	179.12	43.73	42.87	306.00	22.7	23.30	
45	2,5-dimethylheptane	136.00	179.37	43.84	43.87	307.80	22.7	21.30	
46	2,6-dimethylheptane	135.21	180.91	43.92	42.82	306.00	23.7	20.83	-102.90



S.No.	Alkane	bp(°C)	mv(cm ³)	mr(cm ³)	hv(kJ)	ct(°C)	cp(atm)	st(dyne/cm)	mp(°C)
47	3,3- dimethylheptane	137.300	176.897	43.6870	42.66	314.00	24.19	22.01	
48	3,4- dimethylheptane	140.600	175.349	43.5473	43.84	322.70	24.77	22.80	
49	3,5- dimethylheptane	136.000	177.386	43.6379	42.98	312.30	23.59	21.77	
50	4,4- dimethylheptane	135.200	176.897	43.6022	42.66	317.80	24.18	22.01	
51	3-ethyl-2-methylhexane	138.000	175.445	43.6550	43.84	322.70	24.77	22.80	
52	4-ethyl-2-methylhexane	133.800	177.386	43.6472	42.98	330.30	25.56	21.77	
53	3-ethyl-3-methylhexane	140.600	173.077	43.2680	44.04	327.20	25.66	23.22	
54	2,2,4- trimethylhexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51	-120.00
55	2,2,5- trimethylhexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04	-105.78
56	2,3,3- trimethylhexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41	-116.80
57	2,3,4- trimethylhexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80	
58	2,3,5- trimethylhexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27	-127.80
59	3,3,4- trimethylhexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27	-101.20
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75	-33.11
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38	-99.20
62	2,3-dimethyl-3-ethylpentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87	
63	2,4-dimethyl-3-ethylpentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80	-122.20
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38	-99.0
65	2,2,3,4- tetramethylpentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98	-121.09
66	2,2,4,4- tetramethylpentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37	-96.54
67	2,3,3,4- tetramethylpentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31	-102.12



Regression Models

The following statistical models have been used for the study:

- Linear Model: $P = a(\textit{Domination Parameter}) + b$
- Quadratic Model :
 $P = a(\textit{Domination Parameter})^2 + b(\textit{Domination Parameter}) + c$
- Logarithmic Model: $P = a + b \ln(\textit{Domination Parameter})$

where P is a physical property, a, b and c are constants.

Now we have obtained the following different regression models for each domination parameter, which are listed below.

Domination Number $\gamma(G)$

1. Linear Model

$$bp = 1.055 + [\gamma(G)]30.584 \quad (1)$$

$$mv = -0.104 + [\gamma(G)]34.525 \quad (2)$$

$$mr = 0.187 + [\gamma(G)]25.339 \quad (3)$$

$$hv = 0.189 + [\gamma(G)]24.576 \quad (4)$$

$$ct = 1.469 + [\gamma(G)]174.941 \quad (5)$$

$$cp = 42.875 - [\gamma(G)]4.459 \quad (6)$$

$$st = 0.056 + [\gamma(G)]16.714 \quad (7)$$

$$mp = -130.759 + [\gamma(G)]0.367 \quad (8)$$

2. Quadratic Model

$$bp = 3.936[\gamma(G)]^2 - 0.021[\gamma(G)] - 51.675 \quad (9)$$

$$mv = 1.433[\gamma(G)]^2 - 0.006[\gamma(G)] + 92.142 \quad (10)$$

$$mr = 0.437[\gamma(G)]^2 - 0.002[\gamma(G)] + 18.200 \quad (11)$$

$$hv = 0.414[\gamma(G)]^2 - 0.002[\gamma(G)] + 18.144 \quad (12)$$

$$ct = 3.996[\gamma(G)]^2 - 0.019[\gamma(G)] + 102.779 \quad (13)$$

$$cp = -0.200[\gamma(G)]^2 + 0.001[\gamma(G)] + 37.261 \quad (14)$$

$$st = 0.145[\gamma(G)]^2 - 0.001[\gamma(G)] + 14.181 \quad (15)$$

$$mp = 0.979[\gamma(G)]^2 - 0.004[\gamma(G)] - 148.202 \quad (16)$$

3. Logarithmic Model

$$bp = 65.992 - \ln[\gamma(G)]169.477 \quad (17)$$

$$mv = 64.861 + \ln[\gamma(G)]76.576 \quad (18)$$

$$mr = 9.942 + \ln[\gamma(G)]23.165 \quad (19)$$

$$hv = 10.487 + \ln[\gamma(G)]22.253 \quad (20)$$

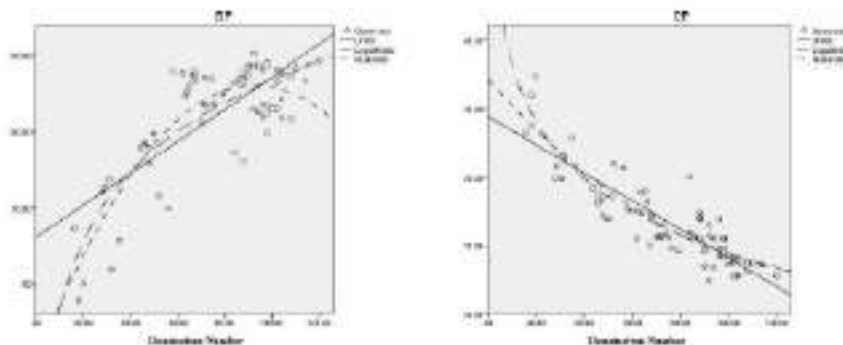
$$ct = 11.075 - \ln[\gamma(G)]8.115 \quad (21)$$

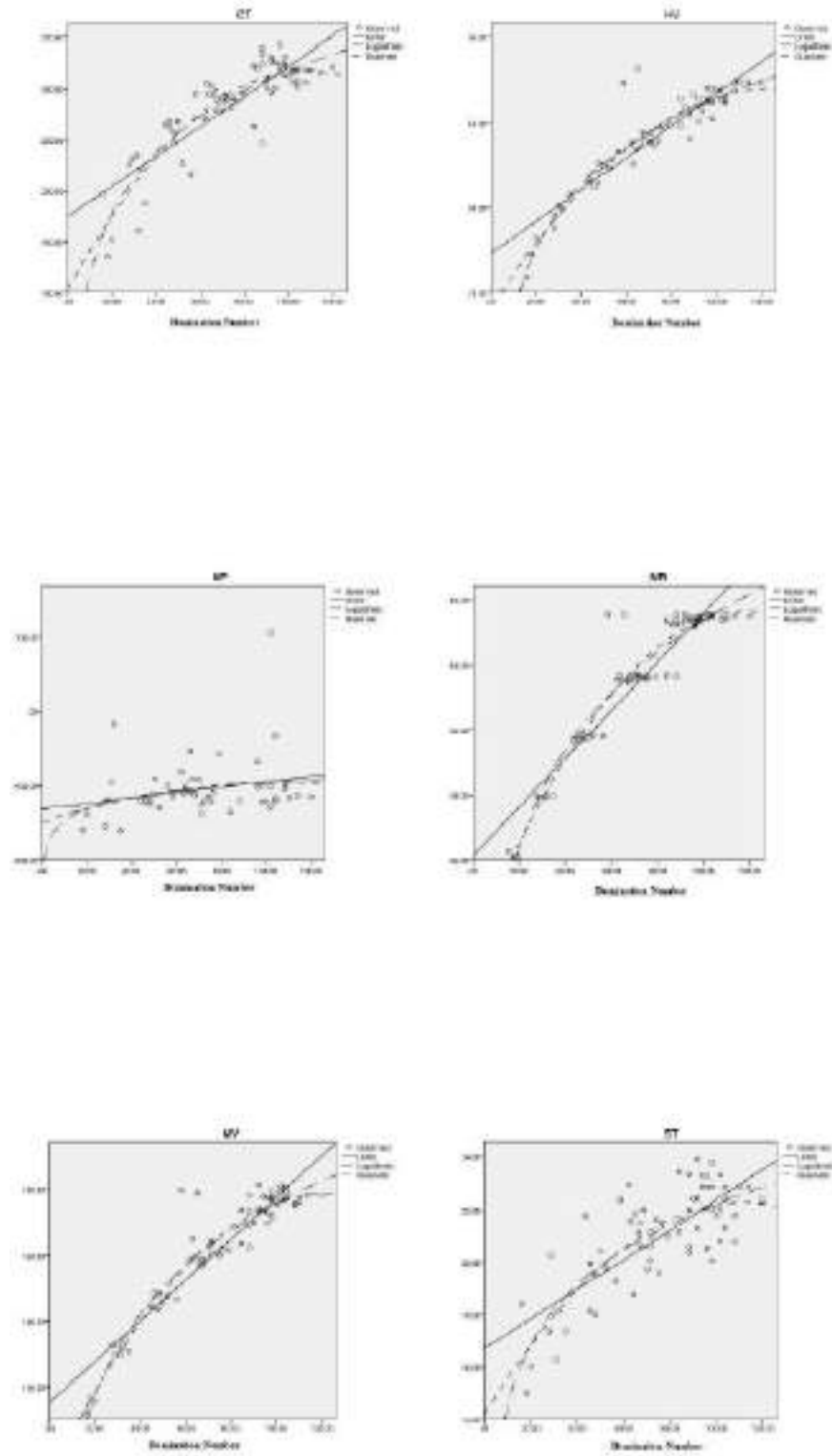
$$cp = -7.067 - \ln[\gamma(G)]52.375 \quad (22)$$

$$st = 11.673 + \ln[\gamma(G)]7.305 \quad (23)$$

$$mp = 22.127 - \ln[\gamma(G)]196.768 \quad (24)$$

In the following figures, the correlation of domination number with above mentioned physical properties of alkanes are shown:





Connected Domination Number $\gamma_c(G)$

1. Linear Model

$$bp = -46.450 + [\gamma_c(G)]0.379 \quad (25)$$

$$mv = 78.533 + [\gamma_c(G)]0.283 \quad (26)$$

$$mr = 10.916 + [\gamma_c(G)]1.412 \quad (27)$$

$$hv = 14.435 + [\gamma_c(G)]2.43 \quad (28)$$

$$ct = 99.561 + [\gamma_c(G)]10.457 \quad (29)$$

$$cp = 28.113 - [\gamma_c(G)]0.235 \quad (30)$$

$$st = 25.256 + [\gamma_c(G)]0.529 \quad (31)$$

$$mp = -174.768 + [\gamma_c(G)]2.436 \quad (32)$$

2. Quadratic Model

$$bp = 10.567[\gamma_c(G)]^2 - 0.884[\gamma_c(G)] - 132.568 \quad (33)$$

$$mv = 7.876[\gamma_c(G)]^2 - 0.143[\gamma_c(G)] + 60.263 \quad (34)$$

$$mr = 3.132[\gamma_c(G)]^2 - 0.052[\gamma_c(G)] + 31.184 \quad (35)$$

$$hv = 3.448[\gamma_c(G)]^2 - 0.075[\gamma_c(G)] + 11.971 \quad (36)$$

$$ct = 36.365[\gamma_c(G)]^2 - 0.625[\gamma_c(G)] + 18.542 \quad (37)$$

$$cp = -7.363[\gamma_c(G)]^2 + 0.047[\gamma_c(G)] + 56.692 \quad (38)$$

$$st = 0.967[\gamma_c(G)]^2 - 0.010[\gamma_c(G)] + 13.482 \quad (39)$$

$$mp = 2.732[\gamma_c(G)]^2 - 0.047[\gamma_c(G)] - 149.022 \quad (40)$$

3. Logarithmic Model

$$bp = -194.741 + \ln[\gamma_c(G)]100.176 \quad (41)$$

$$mv = 9.017 + \ln[\gamma_c(G)]64.949 \quad (42)$$

$$mr = -3.628 + \ln[\gamma_c(G)]19.187 \quad (43)$$

$$hv = -7.376 + \ln[\gamma_c(G)]12.107 \quad (44)$$

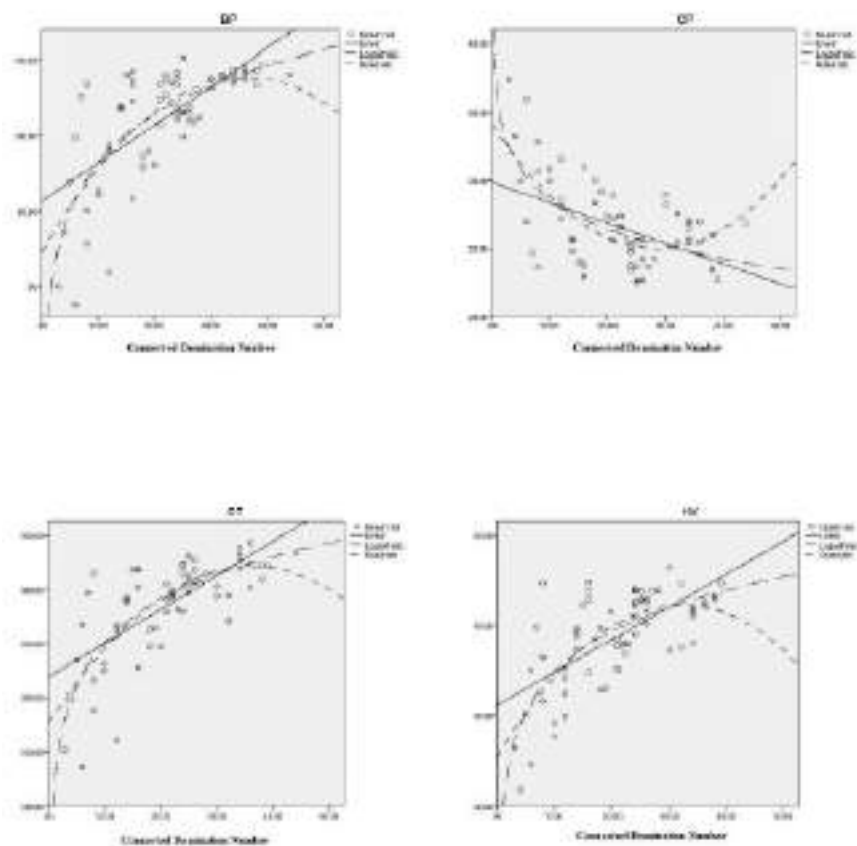
$$ct = -117.478 + \ln[\gamma_c(G)]165.712 \quad (45)$$

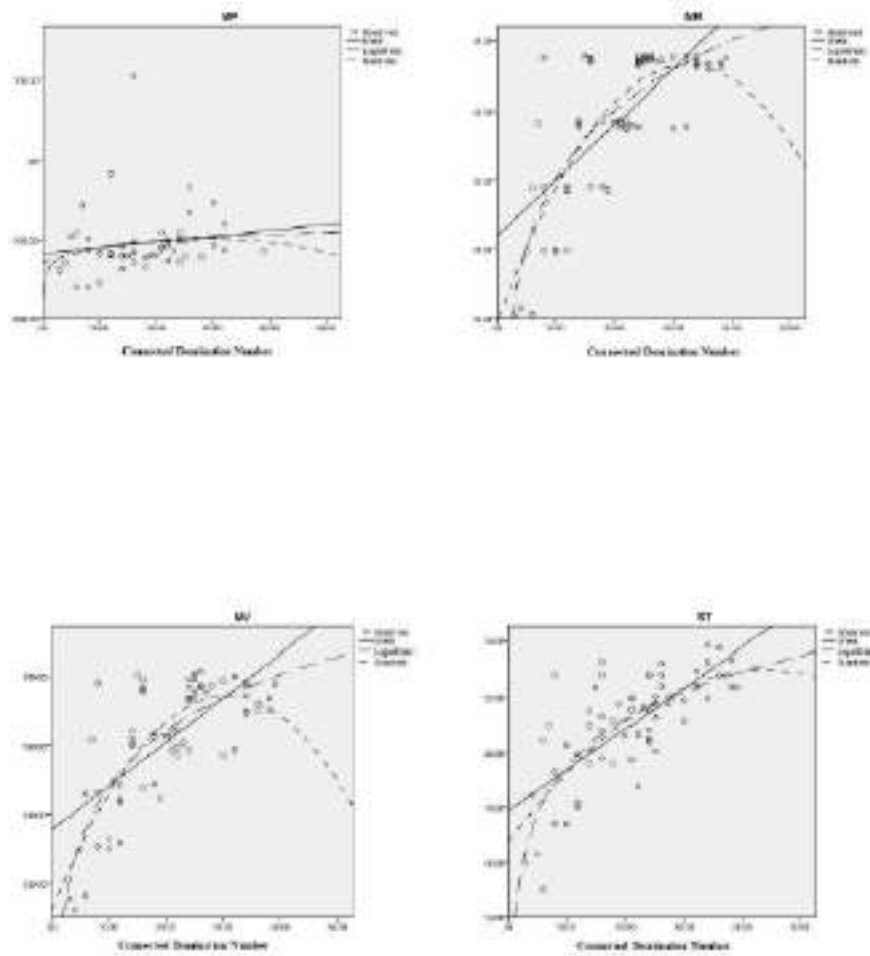
$$cp = 55.929 - \ln[\gamma_c(G)]10.959 \quad (46)$$

$$st = 6.786 + \ln[\gamma_c(G)]7.458 \quad (47)$$

$$mp = -210.472 + \ln[\gamma_c(G)]35.081 \quad (48)$$

In the following figures, the correlation of connected domination number with above mentioned physical properties of alkanes are shown:





Independent Domination Number $\gamma_i(G)$

1. Linear Model

$$bp = 5.194 + [\gamma_i(G)]4,554 \tag{49}$$

$$mv = 107.456 + [\gamma_i(G)]0.870 \tag{50}$$

$$mr = 23.218 + [\gamma_i(G)]1.456 \tag{51}$$

$$hv = 23.909 + [\gamma_i(G)]0.886 \tag{52}$$

$$ct = 123.038 + [\gamma_i(G)]4.317 \tag{53}$$

$$cp = 57.082 - [\gamma_i(G)]0.248 \tag{54}$$

$$st = 13.125 + [\gamma_i(G)]0.578 \tag{55}$$

$$mp = -145.961 + [\gamma_i(G)]1.265 \tag{56}$$

2. Quadratic Model

$$bp = 11.9[\gamma_i(G)]^2 - 0.12[\gamma_i(G)] - 47.612 \quad (57)$$

$$mv = 4.654[\gamma_i(G)]^2 - 0.042[\gamma_i(G)] + 88.216 \quad (58)$$

$$mr = 1.132[\gamma_i(G)]^2 - 0.15[\gamma_i(G)] + 18.132 \quad (59)$$

$$hv = 1.316[\gamma_i(G)]^2 - 0.015[\gamma_i(G)] + 14.259 \quad (60)$$

$$ct = 10.192[\gamma_i(G)]^2 - 0.0101[\gamma_i(G)] + 78.430 \quad (61)$$

$$cp = -0.980[\gamma_i(G)]^2 + 0.014[\gamma_i(G)] + 23.965 \quad (62)$$

$$st = 0.340[\gamma_i(G)]^2 - 0.008[\gamma_i(G)] + 23.456 \quad (63)$$

$$mp = 2.613[\gamma_i(G)]^2 - 0.25[\gamma_i(G)] - 134.608 \quad (64)$$

3. Logarithmic Model

$$bp = -147.275 + \ln[\gamma_i(G)]78.903 \quad (65)$$

$$mv = 45.434 + \ln[\gamma_i(G)]40.210 \quad (66)$$

$$mr = 0.876 + \ln[\gamma_i(G)]10.236 \quad (67)$$

$$hv = 21.608 + \ln[\gamma_i(G)]0.655 \quad (68)$$

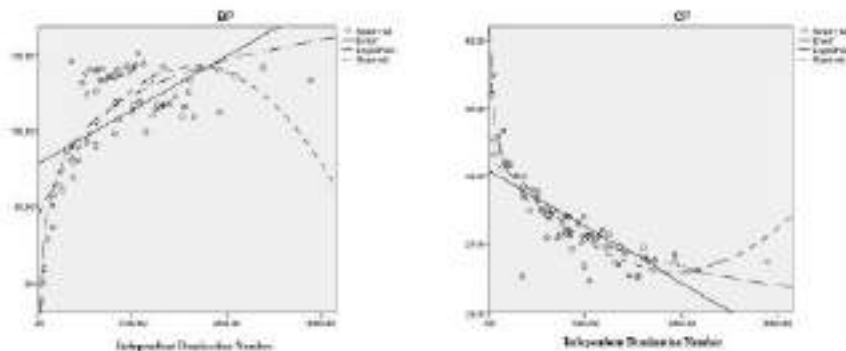
$$ct = -50.591 + \ln[\gamma_i(G)]100.567 \quad (69)$$

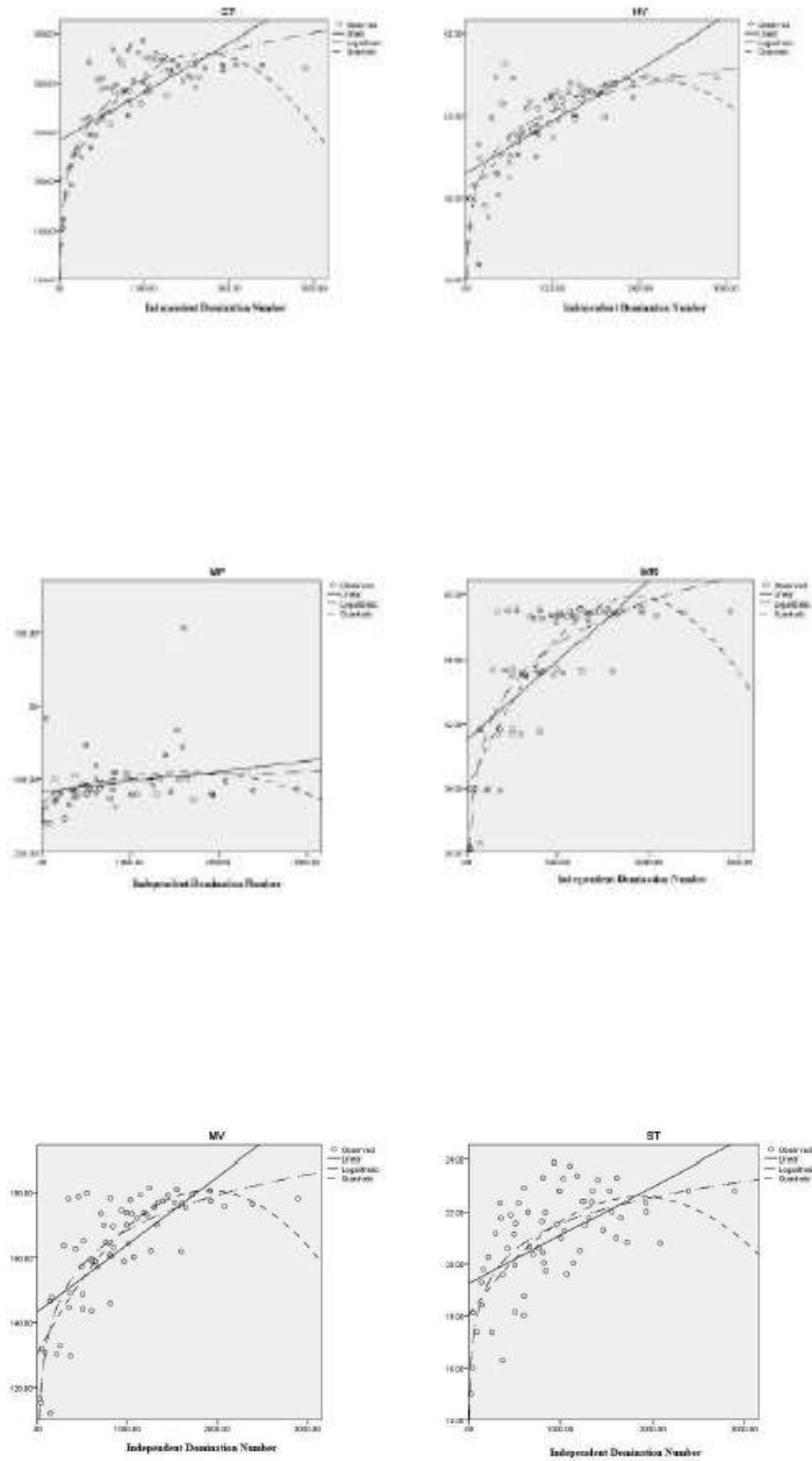
$$cp = 44.853 - \ln[\gamma_i(G)]4.139 \quad (70)$$

$$st = 5.452 + \ln[\gamma_i(G)]3.511 \quad (71)$$

$$mp = -186.817 + \ln[\gamma_i(G)]18.221 \quad (72)$$

In the following figures, the correlation of independent domination number with above mentioned physical properties of alkanes are shown:





Total Domination Number $\gamma_t(G)$

1. Linear Model

$$bp = -56.617 + [\gamma_t(G)]36.785 \quad (73)$$

$$mv = 75.043 + [\gamma_t(G)]13.988 \quad (74)$$

$$mr = 14.070 + [\gamma_t(G)]5.401 \quad (75)$$

$$hv = 16.809 + [\gamma_t(G)]5.912 \quad (76)$$

$$ct = 74.987 + [\gamma_t(G)]35.537 \quad (77)$$

$$cp = 37.578 - [\gamma_t(G)]3.013 \quad (78)$$

$$st = 15.840 + [\gamma_t(G)]2.435 \quad (79)$$

$$mp = -158.005 + [\gamma_t(G)]10.104 \quad (80)$$

2. Quadratic Model

$$bp = 78.544[\gamma_t(G)]^2 - 4.622[\gamma_t(G)] - 168.756 \quad (81)$$

$$mv = 51.766[\gamma_t(G)]^2 - 4.004[\gamma_t(G)] + 14.767 \quad (82)$$

$$mr = 10.465[\gamma_t(G)]^2 - 0.178[\gamma_t(G)] - 1.474 \quad (83)$$

$$hv = 12.506[\gamma_t(G)]^2 - 1.050[\gamma_t(G)] - 4.654 \quad (84)$$

$$ct = 124.251[\gamma_t(G)]^2 - 8.838[\gamma_t(G)] - 110.078 \quad (85)$$

$$cp = -10.902[\gamma_t(G)]^2 + 0.879[\gamma_t(G)] + 56.177 \quad (86)$$

$$st = 3.676[\gamma_t(G)]^2 - 0.253[\gamma_t(G)] + 5.254 \quad (87)$$

$$mp = 12.231[\gamma_t(G)]^2 - 0.881[\gamma_t(G)] - 156.446 \quad (88)$$

3. Logarithmic Model

$$bp = -165.05 + \ln[\gamma_t(G)]132.211 \quad (89)$$

$$mv = 45.460 + \ln[\gamma_t(G)]56.637 \quad (90)$$

$$mr = 0.876 + \ln[\gamma_t(G)]12.235 \quad (91)$$

$$hv = 7.204 + \ln[\gamma_t(G)]16.929 \quad (92)$$

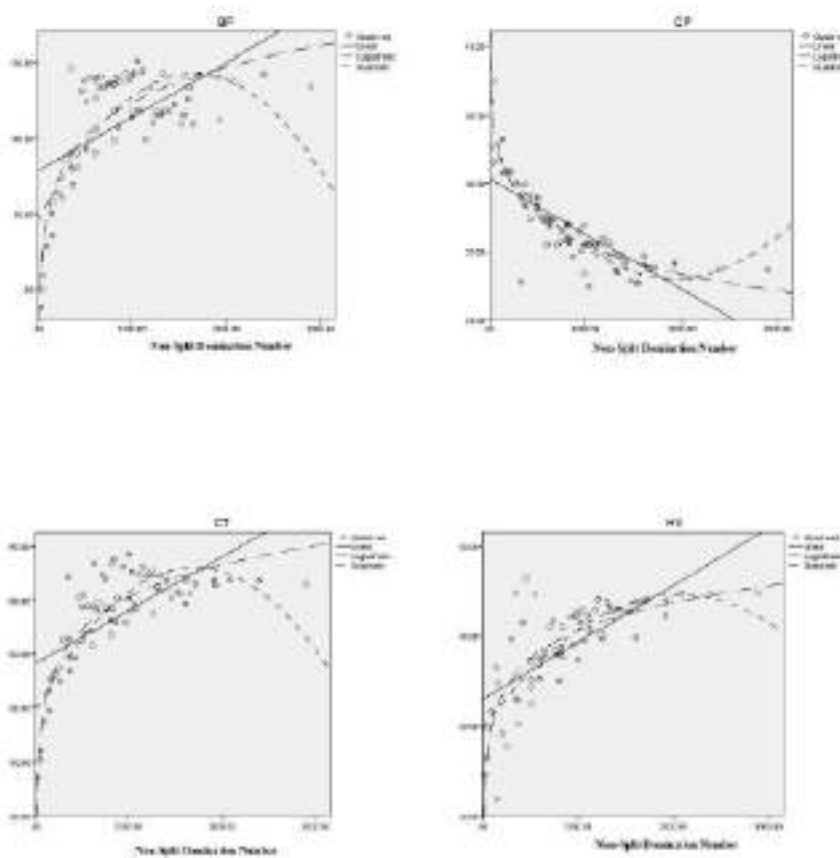
$$ct = -55.591 + \ln[\gamma_t(G)]110.013 \quad (93)$$

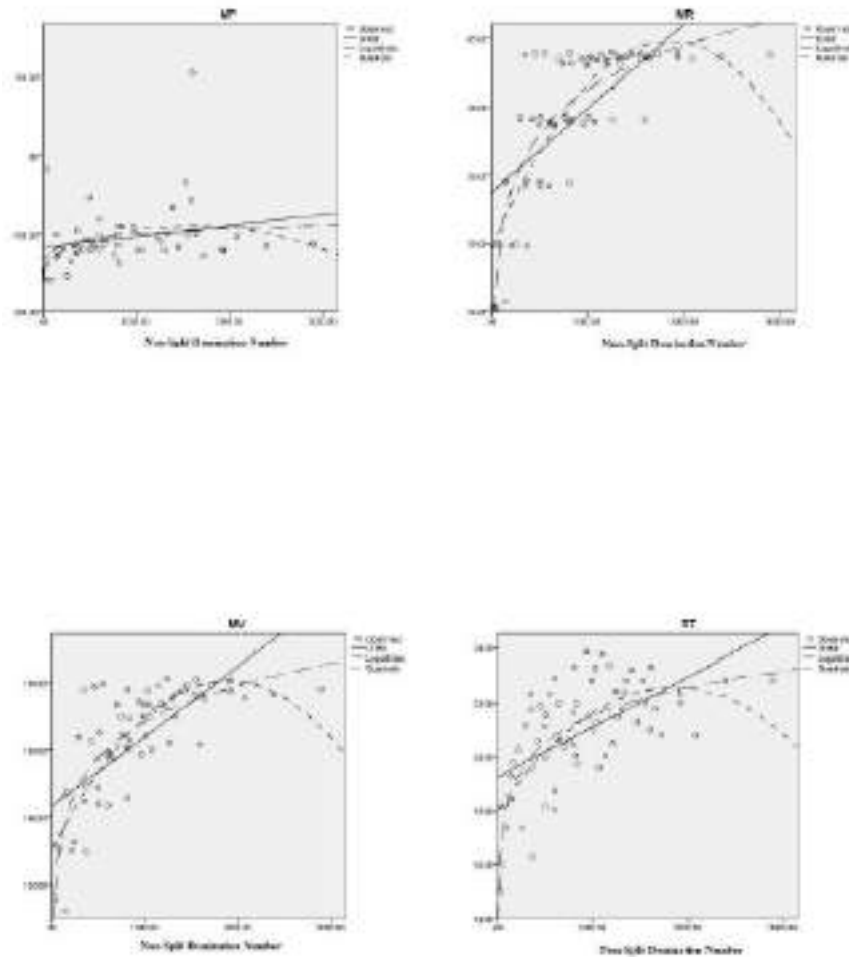
$$cp = 42.629 - \ln[\gamma_t(G)]10.323 \quad (94)$$

$$st = 10.567 + \ln[\gamma_t(G)]4.725 \quad (95)$$

$$mp = -162.589 + \ln[\gamma_t(G)]47.054 \quad (96)$$

In the following figures, the correlation of total domination number with above mentioned physical properties of alkanes are shown:





Split Domination Number $\gamma_s(G)$

1. Linear Model

$$bp = 11.536 + [\gamma_s(G)]1.351 \quad (97)$$

$$mv = 110.932 + [\gamma_s(G)]1.086 \quad (98)$$

$$mr = 30.569 + [\gamma_s(G)]0.213 \quad (99)$$

$$hv = 21.315 + [\gamma_s(G)]0.328 \quad (100)$$

$$ct = 151.329 + [\gamma_s(G)]3.201 \quad (101)$$

$$cp = 32.467 - [\gamma_s(G)]0.280 \quad (102)$$

$$st = 14.205 + [\gamma_s(G)]0.199 \quad (103)$$

$$mp = -131.576 + [\gamma_s(G)]0.276 \quad (104)$$

2. Quadratic Model

$$bp = 5.23[\gamma_s(G)]^2 - 0.036[\gamma_s(G)] - 78.089 \quad (105)$$

$$mv = 1.446[\gamma_s(G)]^2 - 0.008[\gamma_s(G)] + 101.796 \quad (106)$$

$$mr = 0.625[\gamma_s(G)]^2 - 0.001[\gamma_s(G)] + 19.575 \quad (107)$$

$$hv = 0.615[\gamma_s(G)]^2 - 0.001[\gamma_s(G)] + 22.595 \quad (108)$$

$$ct = 6.22[\gamma_s(G)]^2 - 0.035[\gamma_s(G)] + 55.987 \quad (109)$$

$$cp = -0.979[\gamma_s(G)]^2 + 0.002[\gamma_s(G)] + 28.205 \quad (110)$$

$$st = 0.416[\gamma_s(G)]^2 - 0.001[\gamma_s(G)] + 13.182 \quad (111)$$

$$mp = -2.241[\gamma_s(G)]^2 - 0.053[\gamma_s(G)] - 74.870 \quad (112)$$

3. Logarithmic Model

$$bp = -177.566 + \ln[\gamma_s(G)]80.881 \quad (113)$$

$$mv = 27.459 + \ln[\gamma_s(G)]34.302 \quad (114)$$

$$mr = -0.988 + \ln[\gamma_s(G)]10.396 \quad (115)$$

$$hv = 0.359 + \ln[\gamma_s(G)]10.402 \quad (116)$$

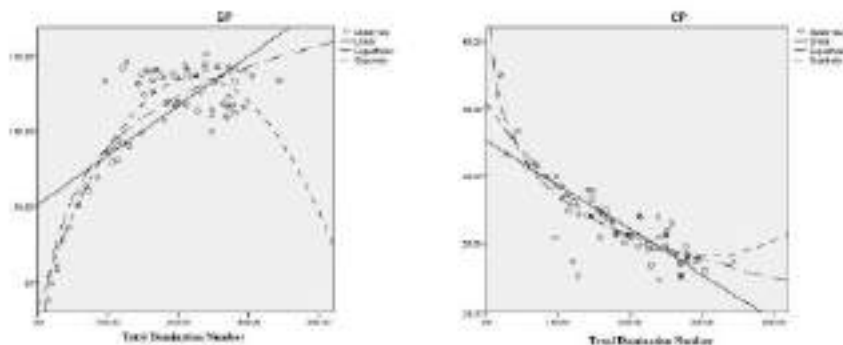
$$ct = -131.812 + \ln[\gamma_s(G)]106.234 \quad (117)$$

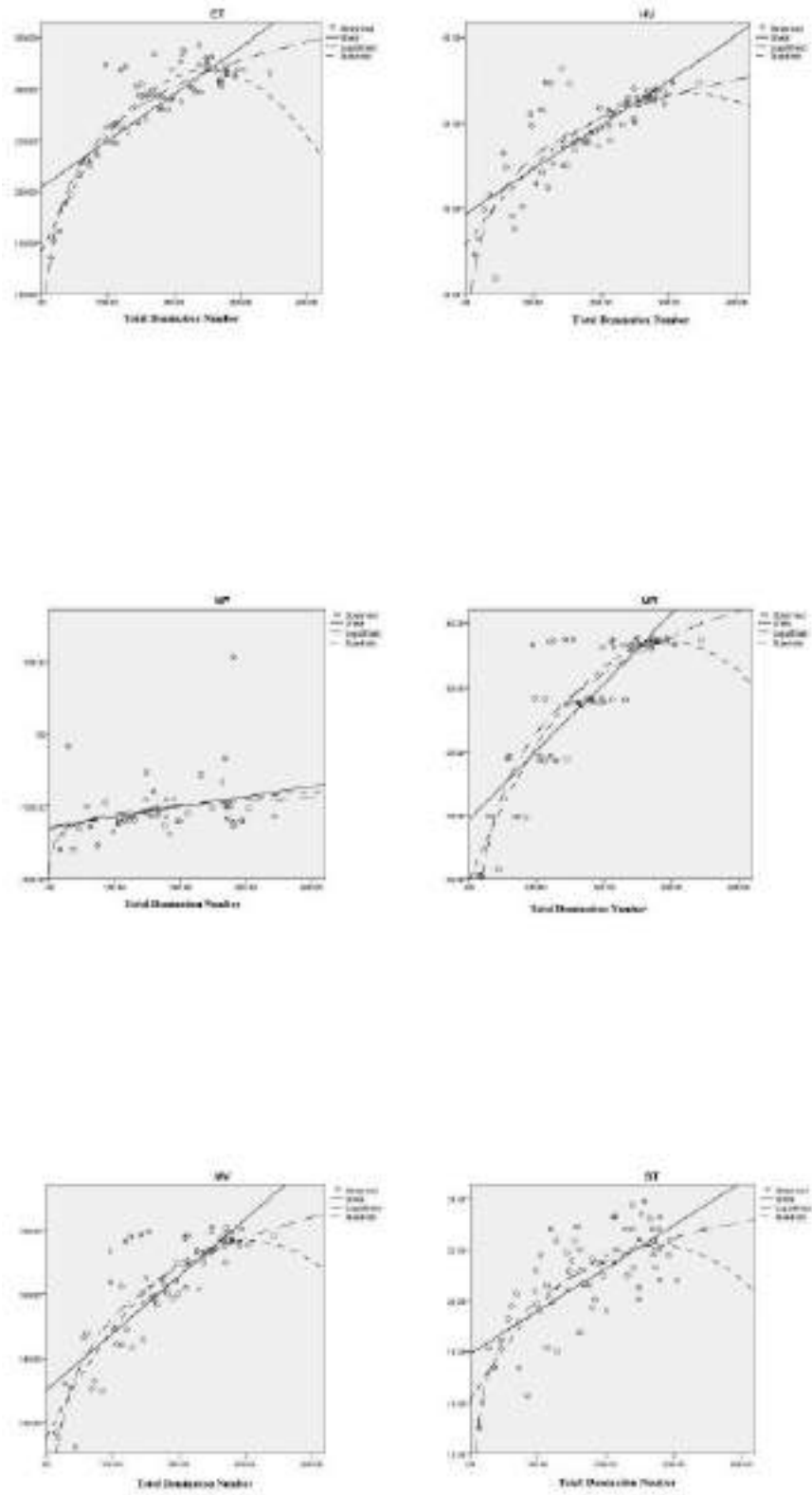
$$cp = 49.847 - \ln[\gamma_s(G)]49.847 \quad (118)$$

$$st = 9.067 + \ln[\gamma_s(G)]3.241 \quad (119)$$

$$mp = -148.213 + \ln[\gamma_s(G)]16.200 \quad (120)$$

In the following figures, the correlation of split domination number with above mentioned physical properties of alkanes are shown:





Non-Split Domination Number $\gamma_{ns}(G)$

1. Linear Model

$$bp = -43.940 + [\gamma_{ns}(G)]24.445 \quad (121)$$

$$mv = 78.145 + [\gamma_{ns}(G)]10.557 \quad (122)$$

$$mr = 17.101 + [\gamma_{ns}(G)]4.777 \quad (123)$$

$$hv = 14.673 + [\gamma_{ns}(G)]2.454 \quad (124)$$

$$ct = 70.271 + [\gamma_{ns}(G)]31.564 \quad (125)$$

$$cp = 39.667 - [\gamma_{ns}(G)]2.102 \quad (126)$$

$$st = 12.563 + [\gamma_{ns}(G)]2.01 \quad (127)$$

$$mp = -149.282 + [\gamma_{ns}(G)]6.457 \quad (128)$$

2. Quadratic Model

$$bp = 82.320[\gamma_{ns}(G)]^2 - 3.141[\gamma_{ns}(G)] - 200.458 \quad (129)$$

$$mv = 10.019[\gamma_{ns}(G)]^2 + 0.123[\gamma_{ns}(G)] + 78.479 \quad (130)$$

$$mr = 3.624[\gamma_{ns}(G)]^2 + 0.013[\gamma_{ns}(G)] + 13.501 \quad (131)$$

$$hv = 2.234[\gamma_{ns}(G)]^2 + 0.061[\gamma_{ns}(G)] + 17.346 \quad (132)$$

$$ct = 61.467[\gamma_{ns}(G)]^2 - 2.567[\gamma_{ns}(G)] - 10.167 \quad (133)$$

$$cp = -3.002[\gamma_{ns}(G)]^2 + 0.078[\gamma_{ns}(G)] + 43.276 \quad (134)$$

$$st = 2.754[\gamma_{ns}(G)]^2 - 0.134[\gamma_{ns}(G)] + 10.012 \quad (135)$$

$$mp = -14.348[\gamma_{ns}(G)]^2 + 1.998[\gamma_{ns}(G)] - 87.176 \quad (136)$$

3. Logarithmic Model

$$bp = -139.117 + \ln[\gamma_{ns}(G)]136.276 \quad (137)$$

$$mv = 42.457 + \ln[\gamma_{ns}(G)]64.795 \quad (138)$$

$$mr = 3.356 + \ln[\gamma_{ns}(G)]18.456 \quad (139)$$

$$hv = 4.367 + \ln[\gamma_{ns}(G)]17.187 \quad (140)$$

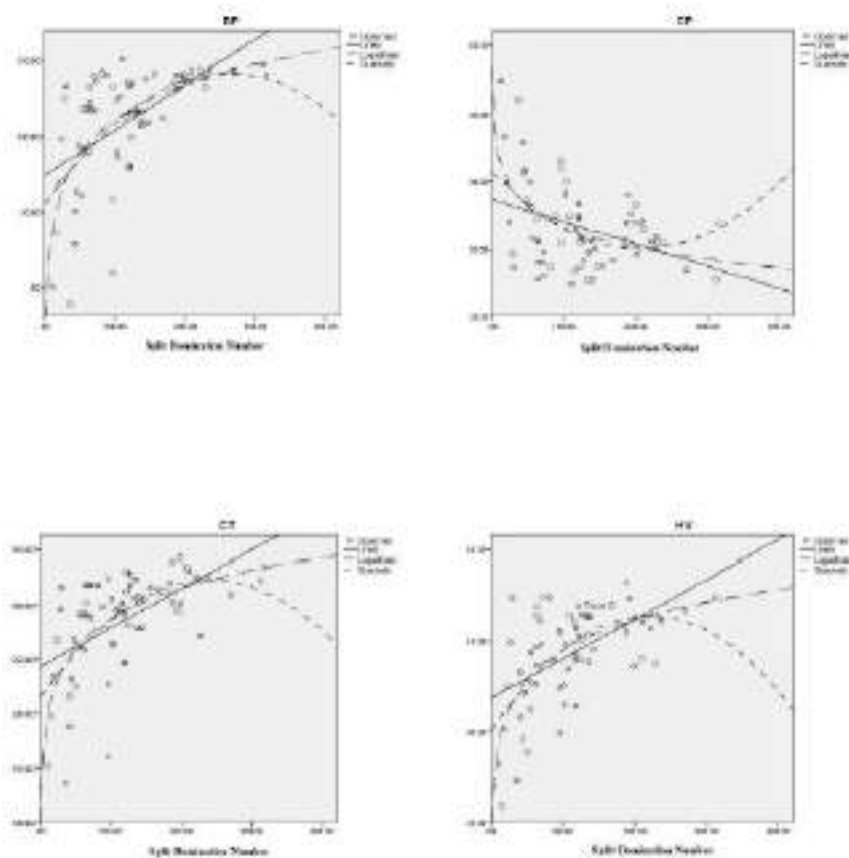
$$ct = -39.742 + \ln[\gamma_{ns}(G)]177.812 \quad (141)$$

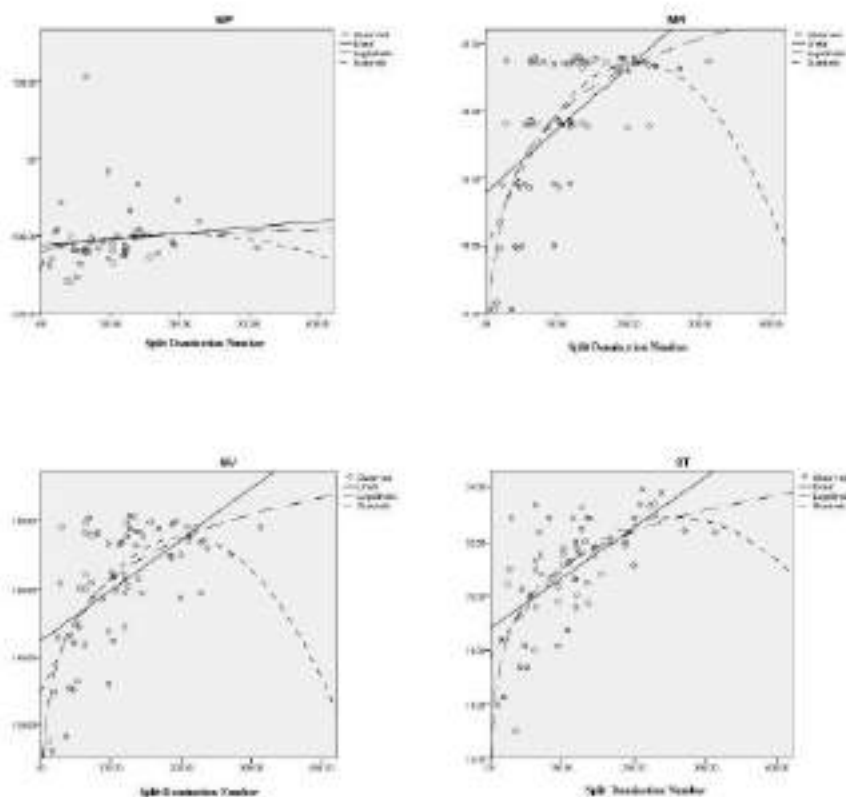
$$cp = 46.467 - \ln[\gamma_{ns}(G)]10.419 \quad (142)$$

$$st = 8.999 + \ln[\gamma_{ns}(G)]7.672 \quad (143)$$

$$mp = -189.470 + \ln[\gamma_{ns}(G)]37.627 \quad (144)$$

In the following figures, the correlation of non-split domination number with above mentioned physical properties of alkanes are shown:





Discussion and Concluding Remarks

By inspection of the data given in tables 1 and 2, and equations (7)-(15) it is possible to draw a number of conclusions for the given domination parameters.

- The domination number $\gamma(G)$ is the first has correlation coefficient value ranging from 0.065 to 0.858 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar volume of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.073 to 0.929 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refraction of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.074 to 0.921 with minimum correlation coefficients value for melting points of alkanes

and maximum correlation coefficient value for molar refraction of alkanes respectively .

- The connected domination number plays an important role in QSPR studies of alkanes. The correlation coefficient value ranges from 0.023 to 0.523 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.029 to 0.626 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.029 to 0.626 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively.
- The independent domination number shows better predicting power than the connected domination number. The correlation coefficient value ranges from 0.054 to 0.596 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical pressure of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.063 to 0.781 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical pressure of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.097 to 0.837 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical pressure of alkanes respectively.
- The total domination number found to be useful parameter in QSPR-studies. The correlation coefficient value ranges from 0.088 to 0.715 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical pressure of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.077 to 0.828 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.089 to 0.832 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.

- The split domination number found to be less useful domination parameter compare to the total domination number. The correlation coefficient value ranges from 0.013 to 0.399 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for surface tension of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.021 to 0.785 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.019 to 0.761 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.
- The non-split domination number has a good predictive power for the set of alkanes. The correlation coefficient value ranges from 0.068 to 0.927 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.080 to 0.463 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.059 to 0.484 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively.

Conclusion.

From practical point of view, topological indices for which the absolute value of correlation coefficient is less than 0.8 can be characterized as useless. Overall, the domination parameters considered for this study are useful candidates to predict the critical temperature of alkanes.

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