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CorrelationofNeighborhoodDominationParameterswithPhysicochemicalPropertiesofn-HeptaneAlkaneIsomers

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Abstract: For each edge e in E, an unordered pair of vertices (u, v) is assigned as the end vertices of e, resulting in a graph G = (V, E). An organic molecule's structure is a basic, non-directed graph. As a result, the vertices of the graph represent molecules, while the edges represent carbon bonds. According to a molecular graph of the n-heptanes alkane isomers, it has been determined that the neighborhood connected dominance number, neighborhood total dominance number, and neighborhood total edge dominance number are all within acceptable ranges. N-heptane alkane isomers' physical attributes are also linked to their neighborhood dominance numbers.
AMSSubjectClassification(2010):05C69

Keywords: Total edge dominance in the neighborhood, neighborhood connected dominance, and neighborhood total edge dominance

1. INTRODUCTION

In this example, let G be a molecular graph that has a vertex set and an edge set. The number of lines that intersect a given vertex's degree, di or degvi, on a graph G. In graph theory, the concept of degree of vertex di is approximately equivalent to the chemical concept of valence [2]. Chemical graphs are mathematical objects that show up for chemical constituents on a periodic table. Mathematical chemistry includes this concept. In addition, it is able to deal with chemical graphs, which represent chemical systems. Thus, the theory of chemical graphs, which deals with the examination of every chemical system connectedness. Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships have found it to be an effective approach [8–11]. Randic [6,7] provide a topological index that has performed well in one of the most QSAR and QSPR investigations involving the above-mentioned topological indices.One of the fastened developed areas in graph theory. It is the study of domination and related

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subsetproblemssuchasindependence,irredundance,coveringandmatching.Anoutstandinghandlingoffundamentals of domination in graphs is specified by the book Haynes et al.,[3]. Surveys of several advancetopics in domination are given in the book edited by Hynes et al.,S. Arumugam et al., mentioned concept ofneighborhood connected domination number [1], D. A. Mojdeh et al., described the definition of neighborhoodtotal domination number [5]. V. R. Kulli introduced the definition for neighborhood total edge dominationnumber[4].Thedefinitions aregivenbelow.

Definition1.1 Consider the graph G = (V, E). A linked graph's dominant set S If the induced subgraph N(S) > of G is connected, it is known as a neighborhood connected dominant set (ncd-set). Neighborhood connected dominating sets are defined by the nc(G) number, which is the smallest cardinality.

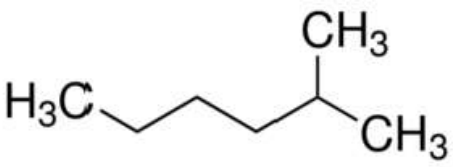
Let G = (V, E) be a graph with no isolated vertices, as defined in Definition1.2. A dominant set S of G is referred to as a

There are no isolated vertices in the induced subgraph N(S) >, hence ntd-set is the neighborhood total dominating set. Neighborhood total domination number (nt(G)) denotes the smallest cardinality of a neighborhood total dominating set (nt(G)).
Definition1.3 Let G=(V, E)be a graph without isolated vertices and isolated edges. An edge dominating set FofGiscalledaneighborhoodtotaledgedominatingsetiftheedgeinducedsubgraph<(F)>hasnoisolatededges.Theneighborhoodtotaledgedominationnumber$\gamma'n(G)$istheminimumcardinality ofneighborhood totaledgedominatingsetof$G$.

Table-I
THEBOILINGPOINT,MELTINGPOINT,HEATFORMATIONOF$C7H16$ISOMERS

C_7H_{16}**Alkane Isomers Names**	**BoilingPoint**	**MeltingPoint**	**Heatformation**
Heptane	98	-91	-44.88
2-methylhexane	90	-118	-41.66
3-methylhexane	92	-119	-41.02
2,2-dimethylpentane	79	-124	-49.27
3,3-dimethylpentane	86	-134	-48.17
2,3-dimethylpentane	90	-104.71	-47.62
2,4-dimethylpentane	81	-119	-48.28
3-ethylpentane	94	-119	-45.33
2,2,3-trimethylbutane	81	-24	-48.95

Example1.1Considerthefollowingfigure



Inabovefigure(2-methylhexane)

Neighborhood Connected Domination number=
4NeighborhoodTotalDominationnumber
=4NeighborhoodTotalEdgeDominatio nnumber=3

2. MAINRESULTSANDDISCUSSION

Domination parameters in the form of neighborhood connected, total, and edge domination numbers are used to understand graph theory in terms of neighborhood domination. Domination parameters for C7H16 structural isomers were discovered through the use of these neighborhood domination parameters, as was a correlation between C7H16 isomer physiochemical qualities and neighborhood dominance parameter domination numbers.

Table-2

SOMENEIGHBORHOODDOMINATIONPARAMETERSVALUESOF$C7H16$STRUCTURALISOMERS

C_7H_{16}**AlkaneIsomersNames**	**Neighborhoodconnecteddominationnumber**N_{γ_c}	**Neighborhoodtotaldominationnumber**N_{γ_t}	**Neighborhoodtotaledgedominationnumber** N_{γ_t}'
Heptane	4	4	4
2-methylhexane	4	4	3
3-methylhexane	5	4	3
2,2-dimethylpentane	5	3	2
3,3-dimethylpentane	4	3	2
2,3-dimethylpentane	4	4	3
2,4-dimethylpentane	5	3	2
3-ethylpentane	4	4	3
2,2,3-trimethylbutane	3	3	2

Table-3

CORRELATION OF DOMINATION PARAMETERS WITH PHYSICOCHEMICAL PROPERTIES OFN-HEPTANE ALKANE ISOMERS

	BoilingPoint	**MeltingPoint**	**HeatFormation**
γ_c	0.235	0.718	0.339
γ_t	0.890	0.161	0.775
γ_t'	0.936	0.041	0.649

Table-4

STATISTICALPARAMETERSBETWEENPHYSICOCHEMICALPROPERTIESANDNEIGHBORHOODCONNECTEDDOMINATIONNUMBER$\gamma n(G)$FORTHELINERQSPRMODEL

Physicochemical Properties	**Correlation(R)**	**Standarderrorof estimate (S)**	**Variance(F)**
BoilingPoint	0.235	6.80	0.411
MeltingPoint	0.718	24.56	7.433
HeatFormation	0.338	3.26	0.781

Table-5.

STATISTICAL PARAMETERS BETWEEN PHYSICOCHEMICAL PROPERTIES ANDNEIGHBORHOODTOTALDOMINATIONNUMBER$\gamma n(G)$FORTHELINERQSPRMODEL

Physicochemical Properties	Correlation(R)	Standarderrorof estimate(S)	Variance(F)
Boiling Point	0.890	3.19	26.546
MeltingPoint	0.161	34.81	0.187
HeatFormation	0.775	2.09	10.530

Table-6.
STATISTICAL PARAMETERS BETWEEN PHYSICOCHEMICAL PROPERTIES ANDNEIGHBORHOODTOTALEDGEDOMINATIONNUMBER$\gamma'n(G)$FORTHELINERQSPR

Physicochemical Properties	R	S	F
BP	0.936	2.46	49.550
MP	0.041	35.244	0.012
HeatFormation	0.649	2.525	5.092

Researchers found that a QSPR research of Neighborhood Connected Domination number Nc can be effective in determining n-Heptane alkane isomer boiling, melting, and heat formation points. As shown in Table-4, the Neighborhood Connected Domination number Nc has a strong link with all C7H16 isomers' physical attributes. Between 0.235 to 0.718, the correlation coefficient between Nc and C7H16 isomers is found. For the melting point of C7H16 alkane isomers, the correlation coefficient of Neighborhood Connected Domination number Nc is high at r = 0.718.

There is a strong association between the Neighborhood Total Domination number Nt and the physical features of C7H16 isomers, as seen in Table-5. C7H16 isomers are correlated with Neighborhood total Domination number nt(G) between 0.161 and 0.890, respectively. For the boiling point of C7H16 alkane isomers, the correlation coefficient of Neighborhood Total Domination number nt(G) is quite strong at r = 0.890.

FromTable-6,itcanbeverifiedeasilythatNeighborhoodtotaledgedominationnumber$\gamma'n(G)$shows

that good correlation with all the physical properties of $C7H16$isomers. The correlation coefficient ofNeighborhood total edge domination number $\gamma'n(G)$ with $C7H16$isomers lies between 0.041 to 0.936. Thecorrelationcoefficientvalueof Neighborhoodtotaledgedominationnumber$\gamma'n(G)$ isveryhighforthe MeltingPointandBoilingPointof$C7H16$alkaneisomerswithr=0.936.

CONCLUSION

Chemists are well aware of the graph dominance. Physicochemical features of C7H16 isomers and Neighborhood domination parameters are correlated in this study. There is a strong association between the two, and it has also been argued whether the dominating parameters give a high or low level. The type of correlation that will occur if the domination parameters are altered is still up for debate.

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