

Contents

List of Figures	xvii
List of Tables	xix
Symbols	xxi
Preface	xxiii
1 Introduction	1
1.1 Graph-Theoretical Concepts	2
1.1.1 Molecular Graphs	3
1.2 Topological Indices	4
1.2.1 Distance-Based Topological Indices	5
1.2.2 Degree-Based Topological Indices	6
1.3 Applications of Topological Indices	9
1.4 Objective of the Thesis	10
1.5 Literature Review	11
1.6 Outline of the Thesis	12
2 Second Reformulated Zagreb Index for Graphs With Cyclomatic Number At Most Three	15
2.1 Introduction	15
2.2 Graph Transformations	15
2.2.1 Graph Transformations to Increase the Index Value	16
2.2.2 Graph Transformations to Decrease the Index Value	29
2.3 Bounds of Second Reformulated Zagreb Index	47
2.3.1 Trees	47
2.3.2 Unicyclic Graphs	47
2.3.3 Bicyclic Graphs	49
2.3.4 Tricyclic Graphs	51
2.4 Summary	54
3 Symmetric Division Deg Index for Trees and Unicyclic Graphs	55
3.1 Introduction	55
3.2 Trees with Perfect Matching	56
3.2.1 Lower Bounds for <i>SDD</i> Index	57
3.2.2 Upper Bounds for <i>SDD</i> Index	59
3.3 Unicyclic Graphs with Perfect Matching	63

3.3.1	Lower Bounds for <i>SDD</i> Index	64
3.3.2	Upper Bounds for <i>SDD</i> Index	66
3.4	Summary	71
4	SDD Index for Bicyclic graphs	73
4.1	Introduction	73
4.1.1	Notations and Definitions	73
4.2	Lower Bounds	74
4.2.1	Subclass β_{2n}^1	74
4.2.2	Subclass β_{2n}^2	78
4.2.3	Subclass β_{2n}^3	80
4.3	Upper Bounds	86
4.4	Summary	95
5	Application of SDD Index	97
5.1	Introduction	97
5.2	Physicochemical Properties	97
5.3	VDB Indices vs Properties of PCB Congeners	98
5.3.1	Statistical Model	98
5.3.2	Results and Data Analysis	99
5.3.3	Predictability Analysis	104
5.4	Summary	105
6	M-Polynomial And VDB Indices	109
6.1	Introduction	109
6.2	Definitions and Required Results	109
6.3	Main Results	111
6.4	Application to Nanotubes	115
6.4.1	HC ₅ C ₇ Nanotubes	116
6.4.2	SC ₅ C ₇ Nanotubes	118
6.4.3	VC ₅ C ₇ Nanotubes	119
6.5	Summary	121
7	AL indices and their Applications	123
7.1	Introduction	123
7.2	Novel AL Indices	124
7.3	Degeneracy of AL Indices	126
7.4	Correlation of AL Indices	127
7.4.1	Linear Regression Model for Octane Isomer	128
7.4.2	Linear Regression Model for PCB Congeners	137
7.5	Summary	146
A	Octane Isomer	157
A.1	Physicochemical Properties of Octane Isomer	157
A.2	AL Indices for Octane Isomer	158
B	PolyChloroBiphenyl Congeners	159
B.1	Physicochemical Properties of PCB Congeners	159
B.2	AL Indices for PCB Congeners	165

Bibliography	171
List of publications	183

List of Figures

1.1	A hydrocarbon and its hydrogen depleted molecular graph representation.	4
2.1	Representation of transformation A .	16
2.2	Representation of transformation B .	17
2.3	Representation of transformation C .	21
2.4	Representation of transformation D .	30
2.5	Representation of transformation E .	32
2.6	Representation of transformation F .	46
2.7	Bicyclic graphs which has no pendant vertices	46
2.8	Some bicyclic graphs which are using in upper bounds	50
2.9	Representation of tricyclic graphs in \mathbb{X}_0^n which has no pendant vertices.	52
2.10	Tricyclic graphs in \mathbb{X}_1^n	52
2.11	Tricyclic graphs which attains the upper bounds	53
3.1	Representative trees from the collection $G_i(m)$, $i = 1, 2, 3, 4$.	57
3.2	Representative trees from the collection $G_5(m)$ and $G_6(m)$.	59
3.3	Collection of trees with m -pendant vertices on $\mathbb{T}(m)$, $m = 4, 5, 6, 7$.	60
3.4	Collection of trees with atmost one vertex of degree 4 in $\mathbb{T}(m)$.	60
3.5	Representative graphs for $\mathbb{C}_a(m), \mathbb{C}_b(m)$.	66
3.6	Collection of unicyclic graph with m -pendant vertices on $\mathbb{U}(m)$ for $m = 4, 5, 6, 7$.	67
3.7	Collection of unicyclic graph with m -pendant vertices on $\mathbb{U}(m)$ for $m = 7$.	68
4.1	Bicyclic graphs.	74
4.2	Representation of graphs corresponding to edge-degree partition $E_i^1(G)$ of bicyclic graphs $F_i^1(2n)$, $i = 1, 2, \dots, 8$ respectively.	75
4.3	Representation of graphs corresponding to edge-degree partition $E_i^3(G)$ of bicyclic graphs in $H_i^3(2n)$, $i = 1, 2, \dots, 12$.	82
4.4	Representation of bicyclic graphs which attains maximum <i>SDD</i> index.	87
4.5	Representation of graphs corresponding to edge-degree partition $E(G)$ of bicyclic graphs $D_2^1(2n), D_3^1(2n), D_2^3(2n), D_3^3(2n)$ respectively.	87
4.6	Bicyclic graphs discussed in Subcase 1.1 and having either 12 or 14 vertices.	88
4.7	Illustration of induction in Case (A).	90
4.8	Illustration for the Case (B)(a).	91
4.9	Illustration for the Case (B)(b).	92
4.10	Illustration for the Case (B)(c).	93
5.1	Correlation of vertex degree based indices with log water solubility ($\log Sw$).	101
5.2	Correlation of vertex degree based indices with octanol-water partition coefficient ($\log P$).	102
5.3	Correlation of vertex degree based indices with the melting point (MP).	103

5.4	Correlation of VDB indices with relative enthalpy of formation (dH_f).	105
5.5	Correlation of vertex degree based indices with log Henry constant ($\log H$).	106
5.6	Experimental versus Expected Value of $\log Sw$ and $\log P$	107
6.1	3-D geometry of nanotubes $HC_5C_7(A)$, $SC_5C_7(B)$ and $VC_5C_7(C)$	115
6.2	Structure of $HC_5C_7[3, 3]$ nanotube.	116
6.3	Structure of $SC_5C_7[p, q]$ nanotube.	118
6.4	Structure of $VC_5C_7[3, 4]$ nanotube	120
7.1	Molecular graph of “2,5,4'-Trichloro-1-1'-biphenyl”.	124
7.2	AL indices Vs Acentric factor of octane isomer.	132
7.3	AL indices Vs entropy of octane isomer.	133
7.4	AL indices Vs Enthalpy of vaporization of octane isomer.	135
7.5	AL indices Vs Standard enthalpy of vaporization of octane isomer.	136
7.16	Experimental versus Expected Value of TSA , $\log Sw$, $\log P$ and $\log Yw$ of PCBs. .	145
7.6	AL indices Vs Total surface area of octane isomer.	147
7.7	AL indices Vs Density of octane isomer.	148
7.8	AL indices Vs total surface area (TSA) of PCBs.	149
7.9	AL indices Vs log water solubility ($\log Sw$) of PCBs.	150
7.10	AL indices Vs relative retation time (RRT) of PCBs.	151
7.11	AL indices Vs octanol-water partition coefficient ($\log P$) of PCBs.	152
7.12	AL indices Vs log water activity coefficient ($\log Yw$) PCB.	153
7.13	AL indices Vs Melting point of PCBs.	154
7.14	AL indices Vs relative enthalpy of formation (dH_f) of PCBs.	155
7.15	AL indices Vs log Henry constant ($\log H$) of PCBs.	156

List of Tables

4.1	Edge-degree partition for graphs in β_{16}^1	88
4.2	Edge-degree partition for graphs in β_{18}^1	89
4.3	Edge-degree partition for graphs in β_{20}^1	89
4.4	Edge-degree partition for graphs in β_{12}^3	93
4.5	Edge-degree partition for graphs in β_{14}^3	94
5.1	The statistical parameters of linear regression fit with correlation coefficient for VDB index and log water solubility ($\log Sw$) are given.	100
5.2	The statistical parameters of linear regression fit with correlation coefficient for VDB index and octanol-water partition coefficient ($\log P$) are given.	100
5.3	The statistical parameters of linear regression fit with correlation coefficient for VDB index and Melting point (MP) are given.	100
5.4	The statistical parameters of linear regression fit with correlation coefficient for VDB index and relative enthalpy of formation (dHf) are given.	104
5.5	The statistical parameters of linear regression fit with correlation coefficient for VDB index and log Henry constant ($\log H$) are given.	104
6.1	Degree based topological indices derived from <i>M-polynomial</i> :	111
6.2	<i>M-Polynomial</i> for more degree based topological indices	115
7.1	Measure of sensitivity of indices for octane isomers and <i>PCB</i> congeners.	126
7.2	The statistical table of linear regression model comparing <i>VDB</i> indices with acentric factor of octane isomers.	130
7.3	The statistical table of linear regression model comparing <i>VDB</i> indices with entropy of octane isomers.	131
7.4	The statistical table of linear regression model comparing <i>VDB</i> indices with enthalpy of vaporization of octane isomer.	134
7.5	The statistical table of linear regression model comparing <i>VDB</i> indices with standard enthalpy of vaporization for octane isomer.	134
7.6	The statistical table of linear regression model comparing <i>VDB</i> indices with the total surface area of octane isomer.	137
7.7	The statistical table of linear regression model comparing <i>VDB</i> indices with density of octane isomer.	137
7.8	The statistical table of linear regression model comparing <i>VDB</i> indices with the total surface area of PCBs.	140
7.9	The statistical table of linear regression model comparing <i>VDB</i> indices with the log-water-solubility of PCBs.	141
7.10	The statistical table of linear regression model comparing <i>VDB</i> indices with the relative retention time of PCBs.	141
7.11	The statistical table of linear regression model comparing <i>VDB</i> indices with the octanol-water-partition coefficient of PCBs.	142

7.12	The statistical table of linear regression model comparing <i>VDB</i> indices with the log-water-activity coefficient of PCBs.	142
7.13	The statistical table of linear regression model comparing <i>VDB</i> indices with the melting point of PCBs.	143
7.14	The statistical table of linear regression model comparing <i>VDB</i> indices with the relative enthalpy of formation of PCBs.	144
7.15	The statistical table of linear regression model comparing <i>VDB</i> indices with the log-Henry constant of PCBs.	144
A.1	Experimental value of physicochemical properties of octane isomers	157
A.2	<i>AL</i> Index value of Octane isomers.	158
B.1	The bold values indicate the expected values of the PCB congeners for log-water solubility and octanol-water partition coefficient while the others are experimental data.	159
B.2	<i>AL</i> Index value of Polychlorobiphenyls (PCBs).	165