

CONTENTS

	page
Chapter 1 – INTRODUCTION AND CHEMICAL RELEVANCE	1
1.1 Reiteration	1
1.2 Motivation	1
1.2.1 General Viewpoints	1
1.2.2 Alkane Isomers	4
1.3 Cycloarenes	9
1.3.1 The Story of Kekulene Revisited	9
1.3.2 Other Cycloarenes	11
1.3.3 The Story of Kekulene Continues	12
1.4 Annulenes, Annulenoannulenes, and Annulene Derivatives	14
1.5 Antikekulene	14
1.6 Corannulene	15
1.7 Cyclacenes	16
1.8 Buckminsterfullerene	17
1.9 Nomenclature and Coding	18
1.10 Conclusion	18
 Chapter 2 – CLASSIFICATION OF POLYGONAL SYSTEMS, AND SOME ASPECTS OF KEKULÉ STRUCTURES	 19
2.1 Introduction	19
2.2 Classification of Single Coronoids in Relation to Kekulé Structures	20
2.3 Degenerate and Generalized Single Coronoids	24
2.4 Examples of Single Coronoids, and Their Kekulé Structure Counts	25
2.4.1 Regular Single Coronoids	25
2.4.2 Essentially Disconnected Single Coronoids	25
2.4.3 Additional Instructive Examples	27
2.4.4 Irregular Single Coronoids With Isolated Internal Vertices	28
2.5 Survey of Kekulé Structure Counts for Single Coronoids	29
2.5.1 Combinatorial Formulas	29
2.5.2 Algorithm and Annulenoid Kekulé Structures for Primitive Coronoids	32
2.5.3 General Solution Convenient for Computer Programming	34
2.5.4 Supplementary References	40
2.6 Isospectral Single Coronoids	41
2.7 Some Main Classes of Polyhexes	43
2.7.1 Introduction	43
2.7.2 Hexagonal and Trigonal Lattices, and the Dualist	43
2.7.3 Helicenes and Corohelicenes	44

2.7.4 Planarity and Nonplanarity	46
2.8 Examples of Graph—Theoretically Nonplanar Polyhexes	48
2.8.1 Cyclohelices	48
2.8.2 Möbius—Polyhexes	50
2.9 Polygonal Systems	50
2.9.1 Introduction	50
2.9.2 Mono— q —Polyhexes	51
2.9.3 Holes and Polygons	52
2.9.4 Cluster Systems	52
 Chapter 3 – BENZENOIDS, SINGLE CORONOIDS AND MULTIPLE CORONOIDS	 55
3.1 General Considerations, Basic Definitions, and Terminology	55
3.2 Invariants and Relations Between Them	55
3.2.1 Specifications	55
3.2.2 Relations	56
3.2.3 Outer and Inner Perimeters	58
3.3 Additional Definitions, Terminology and Relations	60
3.3.1 Corona Holes	60
3.3.2 Associated Benzenoid and Perforated Benzenoid	62
3.3.3 Naphthalenic Coronoid	63
3.3.4 Extremal Coronoid	64
3.4 First Enumeration Results for Benzenoids and Coronoids	65
3.5 Smallest Multiple Coronoids	67
3.5.1 Introduction	67
3.5.2 Basic Assumptions	67
3.5.3 Algorithm for Construction of Smallest Multiple Coronoids	68
3.5.4 Discussion and Depiction of Forms	72
3.5.5 Pericondensed Smallest Multiple Coronoids	75
3.6 Perfect and Imperfect Extremal Coronoids	75
3.6.1 Introduction	75
3.6.2 Numbers of Hexagons and of Internal Vertices	77
3.6.3 Catacondensed Extremal Coronoids	78
3.6.4 Extension to Pericondensed Extremal Coronoids	80
3.7 Chemical Formulas	84
3.7.1 Introduction and Notation	84
3.7.2 Inequalities for the Formula Coefficients	84
3.7.3 Table of Formulas	85
3.8 Numbers of Isomers	89
3.8.1 Definition and Notation	89
3.8.2 Numerical Values	91

Chapter 4 – INVARIANTS OF SINGLE CORONOIDS	95
4.1 Introduction	95
4.2 Summary of Invariants and Relations Between Them	95
4.2.1 Summary of Relations	95
4.2.2 Connectivity and the Dias Parameter	97
4.3 Maximum Number of Internal Vertices, and Minimum Number of Hexagons	99
4.3.1 Maximum Number of Internal Vertices, and Extremal Single Coronoids	99
4.3.2 Minimum Number of Hexagons	100
4.3.3 Spiral Walk	101
4.3.4 Perforated Polycircumcoronenes	102
4.4 Possible Values of Invariants	103
4.5 Upper and Lower Bounds for Some Invariants	104
4.5.1 General	104
4.5.2 Functions of the Number of Hexagons and of the Number of Internal Vertices	104
4.5.3 Functions of Invariants Other Than the Number of Hexagons and the Number of Internal Vertices	106
4.6 Minimum Number of Vertices of Degree Two, and Maximum Number of Hexagons	109
4.6.1 Minimum Number of Vertices of Degree Two	109
4.6.2 Maximum Number of Hexagons, and Circular Single Coronoids	110
4.6.3 Spiral Walk	110
4.6.4 Detailed Analysis	111
 Chapter 5 – CHEMICAL FORMULAS OF SINGLE CORONOIDS	 115
5.1 Introduction	115
5.2 Terminology	115
5.3 Inequalities in Terms of the Formula Coefficients	116
5.3.1 When is a Given Formula Compatible With a Single Coronoid?	116
5.3.2 Supplementary Inequalities	118
5.4 Circumscribing and Excising	119
5.4.1 Introduction	119
5.4.2 Definitions of Circumscribing and Excising for Coronoids	119
5.4.3 Possibilities of Circumscribing and Excising	120
5.4.4 Generalization for k -Fold Circumscribing and k -Fold Excising	124
5.4.5 Core Coronoids	125
5.4.6 Algebraic Treatment	127
5.4.7 Catacondensed Single Coronoids	130
5.4.8 Naphthalenic Single Coronoids	132
5.5 Extremal Single Coronoids and Some of Their Subclasses	133
5.5.1 Extremal Single Coronoids	133

5.5.2 Circumextremal Single Coronoids	134
5.5.3 Circular Single Coronoids	136
5.6 Extreme Single Coronoids	139
5.6.1 Definition	139
5.6.2 Formula	139
5.6.3 Nonextremal Extreme Single Coronoids	140
5.7 Table of Formulas	143
5.8 Single Coronoid Isomers and Number of Edges	147
 Chapter 6 – FURTHER STUDIES OF THE CHEMICAL FORMULAS OF SINGLE CORONIDS	 151
6.1 Introduction	151
6.2 Ground Forms and Higher Members	151
6.2.1 Introduction	151
6.2.2 Definitions and Preliminary Treatment	152
6.2.3 Perfect and Imperfect Ground Forms	152
6.2.4 Formulas for Perfect Ground Forms and for Higher Members	154
6.2.5 Formulas for Imperfect Ground Forms	158
6.2.6 Depictions	158
6.2.7 Mapping of Formulas	159
6.3 Formula Index	159
6.4 A Property of Circumscribing	164
6.5 Building—Up	165
6.5.1 Introduction and Basic Concepts	165
6.5.2 Fundamental Building—Up Principle	166
6.5.3 Addition Units	168
6.5.4 Application of the Fundamental Building—Up Principle to Isomers	168
6.5.5 Simplified Building—Up Principles	168
6.5.6 Formations Available for Addition	170
6.5.7 Further Deductions	171
 SUPPLEMENT	 175
Introductory Remarks	175
Summary of Formulas and Definitions	175
Conclusion	177
 Chapter 7 – GENERATION AND ENUMERATION OF SINGLE CORONOID ISOMERS	 179
7.1 Tabulation of Complete Data	179
7.1.1 Introduction and Survey	179
7.1.2 Classification According to <i>neo</i> and the Color Excess	179

7.1.3	Classification According to the Corona Holes	179
7.2	Forms	191
7.3	Methods of Generation	201
7.3.1	Introduction	201
7.3.2	Application of the Fundamental Building—Up Principle	201
7.3.3	Perforating Benzenoids	203
7.3.4	Examples and Discussion	208
7.4	Circular Single Coronoids	209
7.4.1	Introduction	209
7.4.2	Methods	211
7.4.3	Sample Analysis	212
7.4.4	Extension to All Circular Single Coronoids	220
7.5	Circular Benzenoids Perforated by Phenylene Hole	223
7.5.1	Introduction	223
7.5.2	The Systems	223
7.5.3	Results of Enumeration	224
7.6	Circular Benzenoids Perforated by Coronene Hole	228
7.6.1	Introduction	228
7.6.2	The Systems	228
7.6.3	Results of Enumeration	229
7.7	Supplementary Enumeration Data	232
Chapter 8 – THEOREMS FOR SINGLE CORONIDS		235
8.1	Introduction	235
8.2	Some Basic Concepts	235
8.2.1	Additions	235
8.2.2	Alternating Cycles	235
8.2.3	Edge Cuts	236
8.3	A Property of Kekulé Structures	238
8.4	Essentially Disconnected Single Coronoids	239
8.4.1	Properties and Lemmas	239
8.4.2	Main Theorem	243
8.4.3	"Essentially Disconnected Coronoids" are Essentially Disconnected	246
8.5	Normal Single Coronoids	251
8.6	Regular Single Coronoids	253
8.6.1	Definition	253
8.6.2	A Criterion for a Single Coronoid to be Regular	253
8.7	Half Essentially Disconnected Single Coronoids	258
8.7.1	Introductory Remark	258
8.7.2	Main Theorem	258
8.7.3	New Definition	261

8.7.4 Example	263
8.8 Kekuléan and Non-Kekuléan Single Coronoids	263
8.8.1 Introduction	263
8.8.2 Old Theorem	264
8.8.3 Additional Basic Concepts and Properties	264
8.8.4 Main Theorem	266
 BIBLIOGRAPHY	 275
 SUBJECT INDEX	 295