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Atlas of Kekulé Valence Structures of Buckminsterfullerene*

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The 12,500 Kekulé valence structures of Buckminsterfullerene C_{60}, of which only 158 are symmetry distinct, show large variation in their forms and characteristics. We display all 158 symmetry distinct Kekulé valence structures which have been classified according to their innate degree of freedom (df), which varies from the maximal value of df = 10 to df = 5. The most important and unique Kekulé valence structure in which CC double bonds are exocyclic to pentagonal faces belongs to df = 10, while there are 36 symmetry distinct Kekulé structures associated with df = 5.

INTRODUCTION

Buckminsterfullerene C_{60}, the first fullerene structure conceptually conceived and subsequently experimentally observed[1] is the central structure of fullerene chemistry that has developed since the discovery of this novel carbon allotrope. It is important to fully explore all aspects of structural and theoretical chemistry involving C_{60}. We have therefore undertaken to construct all distinct Kekulé valence structures of buckminsterfullerene in order to obtain some insights into the diversity of Kekulé structures in C_{60}. It has been noted that polycyclic benzenoid hydrocarbons, including large benzenoid hydrocarbons like the giant benzenoids of K. Müllen and coworkers,[2] show considerable variations in local ring properties,[3,4] which were extracted by a close analysis of their Kekulé valence structures. It stands to reason therefore that an analysis of Kekulé valence structures may similarly offer novel insights on local properties of fullerenes.

Kekulé valence structures of polycyclic conjugated hydrocarbons, which have been until recently only superficially considered as a basis for a qualitative description of such molecules, apparently contain substantial more useful structural information that chemists in the past granted them. In Table I we summarise salient features of Kekulé valence structures that have, in view of the long history of Kekulé valence structures, only recently came to surface. To these »novel« structural features of Kekulé valence structures we can also add the Pauling Bond Orders,[5] with which most readers are quite familiar, and less known but equally important Clar's aromatic π-sextets,[6] with which most of the readers may not be so familiar. There is no doubt that Kekulé valence structures contain highly interesting structural information on conjugated polycyclic systems that has hitherto tended to be mostly overlooked, or not appreciated. Most of the above mentioned »hidden treasures« of Kekulé valence struc-

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* Dedicated to Dr. Edward C. Kirby in happy celebration of his 70th birthday.

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TABLE I. List of »hidden treasures« of Kekulé valence structures

»Hidden Treasure«	Outline	Ref.
Conjugated Circuits	Resonance energy expressed in terms of $4n+2$ and $4n$ circuits within individual Kekulé valence structure in which alternate CC double and CC single bonds	1
Conjugated Circuits	Aromaticity characterized by the presence (or dominant role) of only $4n+2$ conjugated circuits in the set of Kekulé valence structures while anti-aromaticity characterized by presence of $4n$ conjugated circuits	2
Conjugated Circuits	Total number of conjugated circuits equal to $K–1$, where K is the number of Kekulé structures. Significance of this theorem: a single Kekulé structure contains information on all Kekulé valence structures	3
Conjugated Circuits	Local Aromaticity: Analogous to Pauling bond order one makes count of Kekulé structures in which particular benzene rings appear as Kekulé structures of benzene	4
Resonance Graph	Graph with vertices being the set of Kekulé valence structures and edges representing the dominant interaction between the structures	5
Degree of Freedom	The smallest number of C=C bonds in a Kekulé structure that determines the Kekulé structure completely	6
Degree of Freedom	Inverse Clar Problem: Clar structure of benzenoid hydrocarbon is determined by superposition of all Kekulé valence structures of maximal degree of freedom	7
π-Electron Ring Partition	Two π-electrons of CC double bonds are assigned to a ring if not shared by other rings, otherwise C=C bond contributes one π-electron to the ring	8
π-Electron Ring Partition	Representation of polycyclic conjugated hydrocarbon by a single structural (numerical) formula	9
π-Pentagon/Hexagon Ring Partition	π-electrons of CC double bonds are assigned to pentagonal and hexagonal rings of fullerene and averaged over all rings of the same kind	10

Reference in Table I

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tures, as outlined in a recent comprehensive review on aromaticity in polycyclic conjugated hydrocarbons,[7] have been considered and analysed mostly on benzenoid hydrocarbons and few smaller nonbenzenoid systems, which included alternants (like biphenylenes) and nonalternants (azulene, azupyrene, *etc*.). Such studies have shown that there are significant differences in a number of structural properties of benzenoids and nonbenzenoids that have yet to be better understood. For example, in the case of benzenoid hydrocarbons the resonance graph,[8] which is the graph representing dominant interactions among Kekulé valence structures of a system in Valence Bond type calculations, is connected. This means that it is made of a single component. In contrast the resonance graph of nonbenzenoid systems, including biphenylene, is disconnected, that is, it can have two or more components. Similarly, in the case of polycyclic benzenoid hydrocarbons the underlying Kekulé valence structures that contribute towards Clar's structure have all the maximal degree of freedom.[9] This, however, is no longer the case with buckminsterfullerene.[10] The innate degree of freedom[11] (df) of a Kekulé valence structure is given by the smallest number of CC double bonds in a structure which completely determine the locations of all the remaining CC double bonds. It seems therefore that a close examination of Kekulé valence structures of fullerenes may throw more light on the similarities and dissimilarities between benzenoid and nonbenzenoid conjugated systems as well as between the alternant and nonalternant conjugated systems. Fullerenes are nonalternants, and hence in this respect are close to nonalternant conjugated hydrocarbons. In order to facilitate studies of π-electron properties of fullerenes we offer here Atlas of Kekulé valence structures of buckminsterfullerene.

ON CLASSIFICATION OF KEKULÉ VALENCE STRUCTURES

The milestone in the quantitative characterization of fullerenes is the paper of Klein, Schmalz, Hite, and Seitz[12] who reported in 1986 the count of Kekulé valence structures in buckminsterfullerene, which is an astounding 12,500 structures. This is by an order of magnitude greater than would be the number of Kekulé valence structures of typical benzenoid hydrocarbon of similar size. From the early days of Quantum Chemistry, when the Valence Bond method dominated the scene of Theoretical Chemistry in applications to organic compounds, it was generally accepted that the presence of large number of Kekulé valence structures signifies great molecular stability and consequently considerable aromaticity. Thus the presence of numerous Kekulé valence structures in C_{60} was interpreted as a cause of the well known unusual stability of buckminsterfullerene.

The presence of large number of Kekulé valence structures for fullerenes is begging for a close look at them. To facilitate such an analysis consideration of possible classification of Kekulé valence structures seems plausible. Alternative classification schemes for Kekulé valence structures appear to be of possible interest including:

(i) Classification based on the innate degree of freedom of Kekulé valence structures;

(ii) Classification based on kind and type of conjugated circuits present in Kekulé valence structures.

As we will see the notion of the innate degree of freedom leads to fewer classes in comparison with classifications based on the count of conjugated circuits or generalized Fries rule (*vide infra*). We have chosen df as the property used in listing Kekulé valence structures in this Atlas. That among the 12,500 Kekulé valence structures there are only 158 distinct structures has already been established by Babić and Trinajstić.[13] As has been already reported the distributions of 158 symmetry non-equivalent structures into six possible degrees of freedom is as follows:[10]

$$1\ \mathrm{df}_{10} + 2\ \mathrm{df}_{9} + 33\ \mathrm{df}_{8} + 47\ \mathrm{df}_{7} + 39\ \mathrm{df}_{6} + 36\ \mathrm{df}_{5}$$

Variations in the count of conjugated circuits are considerable even among Kekulé valence structures of the same degree of freedom (Table II). Conjugated circuits are defined within individual Kekulé valence structure as circuits in which there is regular alternation of CC double and CC single bonds.[14,15] They are of $4n$+2 or $4n$ size designated as R_n and Q_n respectively. The smallest $4n$+2 conjugated circuits (6-π electron conjugated circuits) make the dominant contribution to molecular resonance energy. In the case of Kekulé valence structure of buckminsterfullerene the maximal number of the smallest conjugated circuits R_1, which is 20, characterizes the unique Kekulé valence structures of df_{10}. On the other hand numerous Kekulé valence structures have few R_1 conjugated circuits and seven of 158 structures have no R_1 conjugated circuits at all. Besides thus making negligent or no significant contribution to the molecular resonance energy (RE), these structures could not be part of the dominant component of the resonance graph. In Table II we have summarized the count of R_1 in different Kekulé valence structures. In contrast the count of disjoint R_1 conjugated circuits, which are fewer, the maximal number being eight, is of importance when considering the innate degree of freedom and the Clar structures of C_{60}.

In the case of nonbenzenoid systems one may consider classification of Kekulé valence structures based on whether they possess the smallest (and the most important for molecular stability) conjugated circuits R_1 or not. In Figure 1 we show for several nonbezenoid systems their R_1-deficient Kekulé valence structures. It is interesting to see that kekulene, which is built from fused benzene rings also has a Kekulé valence structure with no R_1 conjugated circuits (shown in Figure 2).

Fullerenes belong to nonalternant polycyclic conjugated systems and thus could be expected to have R_1-deficient Kekulé structures. The consequence of R_1-deficient Kekulé valence structures is that resonance graphs become disconnected. This allows one to classify (or associate) Kekulé structures with various components of the disconnected resonance graph. In the case of Buckminsterfullerene one finds that the resonance graph has a single dominant R_1-component that has 5828 vertices. All these 5828 Kekulé valence structures, as elaborated by Flocke, Schmalz, and Klein,[16] can be obtained from the #1 Kekulé valence structure of C_{60} (which has 20 R_1 conjugated circuits and in which all CC double bonds are exocyclic to the twelve pentagonal faces of C_{60}). The 5828 structures were obtained from the structure #1 by rotating CC double bonds within one or more benzene rings. Moreover these authors have shown that by using this smaller set of 5828 Kekulé valence structures (instead of the complete set of 12,500 Kekulé valence structures) they have been able to recover 99.82 % of the energy of the full set in *ab initio* calculations based on Heisenberg model Hamiltonian. Hence over half of Kekulé valence structures of Buckminsterfullerene are practically irrelevant when one is computing molecular energy.

The 5828 Kekulé valence structures of C_{60}, as has been discussed in a review on aromaticity in polycyclic conjugated hydrocarbons,[17] can be partitioned as follows:

$$5\ A_8 + 320\ A_7 + 1240\ A_6 + 1912\ A_5 + 1510\ A_4 + 660\ A_3 + 160\ A_2 + 20\ A_1 + A_0$$

where A_k stands for the number of independent π-aromatic sextets. The partition corresponds to enumeration of the generalized Clar structures in C_{60}, there being five »proper« Clar structures of C_{60}, as has been shown first by El-Basil.[18]

TABLE II. The count of conjugated circuits involving 6, 10 and 14 π-electrons for 158 symmetry non-equivalent Kekulé valence structures of C_{60}, their symmetry weights and the average values for the partitioning of π-electrons to hexagonal and pentagonal faces of C_{60}

Structure	R_1	R_2	R_3	Weight	Hexagons	Pentagons
1	20	0	0	1	3.000	0.000
2	17	3	0	20	2.850	0.250
3	15	4	1	60	2.700	0.500
4	11	6	3	120	2.400	1.000
5	10	5	5	12	2.250	1.250
6	10	5	5	60	2.250	1.250
7	11	7	1	120	2.400	1.000
8	10	6	3	60	2.250	1.250
9	12	7	1	120	2.550	0.750
10	12	7	1	120	2.550	0.750
11	12	7	1	60	2.550	0.750
12	11	6	3	120	2.400	1.000
13	10	8	2	30	2.400	1.000
14	12	7	1	60	2.550	0.750
15	11	6	3	120	2.400	1.000
16	13	5	2	120	2.550	0.750
17	9	7	4	120	2.250	1.250
18	10	8	2	120	2.400	1.000
19	10	5	5	120	2.250	1.250
20	12	4	4	30	2.400	1.000
21	9	4	7	60	2.100	1.500
22	8	6	6	20	2.100	1.500
23	8	9	3	40	2.250	1.250
24	11	6	3	40	2.400	1.000
25	8	6	6	60	2.100	1.500
26	8	3	9	40	1.950	1.750
27	8	0	12	5	1.800	2.000
28	13	6	0	20	2.550	0.750
29	14	6	0	60	2.700	0.500
30	14	6	0	30	2.700	0.500
31	14	6	0	10	2.700	0.500
32	11	6	3	60	2.400	1.000
33	11	9	0	40	2.550	0.750
34	8	12	0	10	2.400	1.000
35	10	0	0	6	2.500	0.833
36	13	5	2	60	2.550	0.750
37	10	8	2	60	2.400	1.000
38	8	6	6	120	2.100	1.500
39	9	7	4	120	2.250	1.250
40	8	9	3	120	2.250	1.250
41	9	7	4	120	2.250	1.250
42	9	7	4	120	2.250	1.250
43	8	9	3	120	2.250	1.250
44	9	10	1	120	2.400	1.000
45	10	8	2	60	2.400	1.000
46	7	2	1	60	2.200	1.333
47	8	10	1	60	2.250	1.250
48	9	8	2	120	2.250	1.250
49	8	7	4	60	2.100	1.500
50	10	8	2	120	2.400	1.000
51	10	8	2	60	2.400	1.000
52	8	6	6	120	2.100	1.500
53	10	8	2	60	2.400	1.000
54	10	8	2	120	2.400	1.000
55	7	9	3	120	2.100	1.500
56	8	7	4	60	2.100	1.500
57	9	7	4	60	2.250	1.250
58	8	7	4	120	2.100	1.500
59	7	6	6	120	1.950	1.750
60	7	6	6	60	1.950	1.750
61	8	6	6	60	2.100	1.500
62	9	7	4	120	2.250	1.250
63	7	7	4	60	1.950	1.750
64	7	6	6	40	1.950	1.750
65	8	7	4	120	2.100	1.500
66	9	8	2	120	2.250	1.250
67	8	2	0	120	2.350	1.083
68	8	2	0	60	2.350	1.083
69	10	9	0	60	2.400	1.000
70	10	9	0	20	2.400	1.000
71	8	10	1	120	2.250	1.250
72	5	0	0	60	2.150	1.417
73	7	3	0	60	2.350	1.083
74	10	0	0	30	2.500	0.833
75	9	8	2	60	2.250	1.250
76	9	8	2	120	2.250	1.250
77	7	9	3	40	2.100	1.500
78	7	9	3	120	2.100	1.500
79	8	7	4	120	2.100	1.500
80	11	9	0	60	2.550	0.750
81	9	7	4	120	2.250	1.250
82	8	8	2	30	2.100	1.500
83	10	8	2	60	2.400	1.000
84	4	4	2	30	1.900	1.833
85	5	4	0	60	2.050	1.583
86	6	4	0	60	2.200	1.333
87	6	4	0	120	2.200	1.333
88	7	2	1	120	2.200	1.333
89	6	4	0	120	2.200	1.333
90	6	4	0	60	2.200	1.333

TABLE II. continued

Structure	R_1	R_2	R_3	Weight	Hexagons	Pentagons
91	8	2	0	120	2.350	1.083
92	5	5	0	120	2.200	1.333
93	3	2	0	120	2.000	1.667
94	6	4	0	60	2.200	1.333
95	6	4	0	30	2.200	1.333
96	5	4	1	120	2.050	1.583
97	3	2	0	120	2.000	1.667
98	6	4	0	60	2.200	1.333
99	4	4	2	60	1.900	1.833
100	5	4	1	120	2.050	1.583
101	4	4	2	120	1.900	1.833
102	6	12	0	10	2.100	1.500
103	6	4	0	60	2.200	1.333
104	3	2	0	60	2.000	1.667
105	5	0	0	60	2.250	1.250
106	4	0	0	30	2.200	1.333
107	4	0	0	60	2.150	1.417
108	0	0	0	6	2.000	1.667
109	6	3	1	120	2.200	1.333
110	0	0	0	30	1.800	2.000
111	0	0	0	10	1.800	2.000
112	5	3	2	120	2.050	1.583
113	5	4	1	120	2.050	1.583
114	4	4	2	60	1.900	1.833
115	5	4	1	120	2.050	1.583
116	6	3	1	120	2.200	1.333
117	5	4	1	120	2.050	1.583
118	5	3	2	120	2.050	1.583
119	7	2	1	60	2.200	1.333
120	4	4	2	30	1.900	1.833
121	2	2	1	60	1.950	1.750
122	5	4	1	120	2.050	1.583
123	4	4	2	60	1.900	1.833
124	4	4	2	60	1.900	1.833
125	2	1	1	120	1.850	1.917
126	3	2	0	60	2.100	1.500
127	2	2	1	120	1.850	1.917
128	5	4	1	120	2.050	1.583
129	5	4	1	120	2.050	1.583
130	5	4	1	60	2.050	1.583
131	4	5	1	120	2.050	1.583
132	2	2	0	60	1.900	1.833
133	2	2	0	60	1.900	1.833
134	3	1	0	120	2.050	1.583
135	1	1	0	120	1.850	1.917
136	0	0	0	30	2.000	1.667
137	0	0	0	60	1.900	1.833
138	2	2	0	60	1.850	1.917
139	2	0	0	20	2.100	1.500
140	4	5	1	120	2.050	1.583
141	0	0	0	60	1.800	2.000
142	2	2	1	120	1.850	1.917
143	0	0	0	60	1.900	1.833
144	2	0	0	60	2.000	1.667
145	2	2	1	120	1.950	1.750
146	4	3	3	120	1.900	1.833
147	3	2	0	120	2.100	1.500
148	5	3	2	120	2.050	1.583
149	3	1	0	120	2.000	1.667
150	2	0	0	20	1.800	2.000
151	2	0	0	40	1.950	1.750
152	2	2	1	60	1.850	1.917
153	6	4	0	60	2.200	1.333
154	4	3	3	120	1.900	1.833
155	2	2	1	120	1.950	1.750
156	4	4	1	120	1.900	1.833
157	3	2	0	120	2.100	1.500
158	2	2	0	120	2.000	1.667

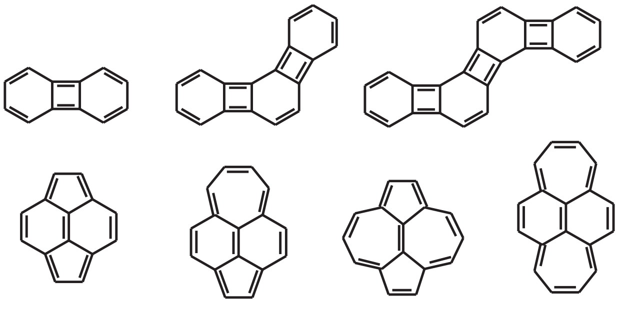

Figure 1. Kekulé structures of various nonbenzenoid systems lacking R_1 conjugated circuits.

ON FRIES VALENCE STRUCTURES

A close look at many benzenoid hydrocarbons has lead to realization that »not all Kekulé valence structures are equal,« that is, equally important. Systematic and close analysis has led Clar to advance his π-Aromatic Sextet model,[3] which essentially asserts that some Kekulé valence structures are more important than others, and suffice when considering alone to adequately account for similarities and differences between various local and global properties of numerous benzenoid hydrocarbons. That some Kekulé valence structures are dominant has been

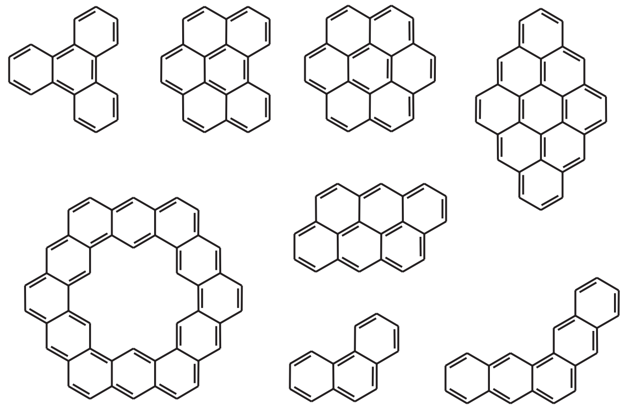

Figure 2. Anti-Fries structures of a selection of smaller benzenoid hydrocarbons including kekulene.

already suggested in 1927 (pre-Quantum Chemistry era) by Fries,[19] who formulated a rule for identifying these most important structures, known as Fries rule (*vide infra*). Logically one should then expect that some Kekulé valence structures are the least important. Such are the Kekulé valence structures shown in Figure 2 belonging to a dozen smaller benzenoid hydrocarbons, referred to as anti-Fries structures.[20] Let us formally define Fries structures and anti-Fries structures for benzenoid hydrocarbons:

(i) Fries structure is the Kekulé valence structure of a benzenoid hydrocarbon which has the largest number of rings with three CC double bonds;

(ii) Anti-Fries structure is the Kekulé valence structure of a benzenoid hydrocarbon which has the smallest number of rings with three CC double bonds.

The underlying idea behind Fries rules is to select a single dominant Kekulé valence structure for a molecule (if possible). Both definitions however allow a possibility that more than one Kekulé valence structure of a benzenoid hydrocarbon qualifies as Fries or anti-Fries structure. It would be nice if indeed one can represent polycyclic conjugated systems, including fullerenes, by a single valence structure that would at the same time be faithful. It was only very recently demonstrated that indeed one can arrive at a single faithful (numerical) representative valence structures for polycyclic conjugated hydrocarbons. Such structures are obtained by superposition of all *numerical* Kekulé valence structures.[21] Numerical Kekulé valence structures have been only very recently introduced. They are obtained by partitioning of π-electron rings to individual benzene rings and by subsequent averaging of all such partitions over all Kekulé valence structures. Thus indeed the »dream« of having a unique structural formula for any benzenoid hydrocarbons has been eventually fulfilled in a form of a single numerical Kekulé valence structure – an accomplishment that has yet to be widely appreciated.

If classification of Kekulé valence structures of fullerenes is to be based on the notion of Fries and Anti-Fries valence structures we have to generalize these two concepts to include Kekulé valence structures »in-between.« One possibility is to use the count of R_1 conjugated circuits as the key structural element (ignoring the presence of other conjugated circuits). Let us designate with F_k the number of Kekulé valence structures having k smallest conjugated circuits R_1. Then the 158 symmetry non equivalent Kekulé valence structures of C_{60} partition as follows:

$$F_{20} + F_{17} + F_{15} + 3F_{14} + 3F_{13} + 5F_{12} + 8F_{11} + 17F_{10} + 13F_9 + 22F_8 + 11F_7 + 12F_6 + 16F_5 + 14F_4 + 8F_3 + 15F_2 + F_1 + 7F_0$$

In total we have 18 classes of Kekulé valence structures. The coefficients in the above expression were obtained from the column R_1 of Table II by adding the occurrence of conjugated circuits involving 6 π-electrons for 158 symmetry non-equivalent Kekulé valence structures of C_{60}.

PARTITION OF π-ELECTRONS TO FIVE- AND SIX-MEMBER RINGS

We included in Table II the average partition of π-electrons to pentagonal faces and hexagonal faces of C_{60}, the two entries being simply related: 20 (π-six ring content) + 12 (π-five ring content) = 60. The resulting numbers are quite interesting as they offer an alternative insight into the distribution of π-electrons in individual Kekulé valence structures. Apparently there is only a rather qualitative correlation between the decrease of the π-electron contributions in the six-member rings and the decrease in the number of R_1 conjugated circuits contributing to the molecular resonance energy, which is summarized in Table III. As we can see from Table III, in which we arranged the Kekulé valence structures of C_{60} according to the average π-electron content of benzene rings, there is considerable variation in the count of R_1 conjugated circuits among valence structures having the same average π-electron content of hexagonal rings.

ATLAS OF KEKULÉ VALENCE STRUCTURES

In the Appendix we show all the 158 distinct Kekulé valence structures of buckminsterfullerene, arranged according to their degree of freedom. At each structure we have also indicated the sequential numbers used in Table II and Table III, which are dictated by our algorithm for construction of Kekulé valence structures (outlined in Ref. 21). However, for all practical matters the ordering of Kekulé structures within each class having the same df in this Atlas can be viewed as arbitrary. It would be of interest to associate generation of Kekulé structures with some orderly algorithm. Orderly algorithms have received attention in Graph Theory[22] and Chemical Graph Theory.[23] They imply or produce canonical labels for structures, thus pointing to a need for canonical labelling of

TABLE III. The distribution of R_1 conjugated circuits for different average population of hexagons with π-electrons

hexagons	R_1	Structure
3.00	20	1
2.85	17	2
2.70	15	3
	14	29, 30, 31
2.55	13	16, 28, 36
	12	9, 10, 11, 14, 20
	11	33, 80
2.50	10	35, 74
2.40	11	4, 7, 12, 15, 24, 32
	10	13, 18, 37, 45, 50, 51, 53, 54, 69, 70, 83
	9	44
	8	34
2.35	8	67, 68, 91
	7	73
2.25	10	5, 6, 8, 19
	9	17, 39, 41, 42, 48, 57, 62, 66, 75, 76, 81
	8	23, 40, 43, 47, 71
	5	105
2.20	7	46, 88, 119
	6	86, 87, 89, 90, 94, 95, 98, 103, 109, 116, 153
	5	92
	4	106
2.15	5	72
	4	107
2.10	9	21, 49
	8	22, 25, 38, 52, 56, 58, 61, 65, 79, 82
	7	55, 77, 78
	6	102
	3	126, 147, 157
	2	139
2.05	5	85, 96, 100, 112, 113, 115, 117, 118, 122, 128, 129, 130, 148
	4	131, 140
	3	134
2.00	3	93, 97, 104, 149
	2	144, 158
	0	108, 136
1.95	8	26
	7	59, 60, 63, 64
	2	121, 145, 151, 155
1.90	4	84, 99, 101, 114, 120, 123, 124, 146, 154, 156
	2	132, 133
	0	137, 143
1.85	2	125, 127, 138, 142, 152
	1	135
1.80	8	27
	2	150
	0	110, 111, 141

Kekulé valence structures, rather than limiting attention solely to partial ordering of Kekulé valence structures – a topic that apparently has received some attention in the chemical literature.[24] In this respect we should mention the recent attempt of Miličević, Nikolić, and Trinajstić to introduce complete order on Kekulé valence structure of benzenoid hydrocarbons.[25]

CONCLUDING REMARKS

The main aim of this communication has been to present pictorially all the distinct Kekulé valence structures of C_{60}. In doing this we also reported tabular information on the count of the smallest (4*n*+2) conjugated circuits (R_1, R_2 and R_3 having 6, 10 and 14 π-electrons, respectively), the innate degrees of freedom of individual Kekulé structures, the average partition of π-electrons between the hexagonal and pentagonal faces of C_{60}, and the distribution of R_1 conjugated circuits for different average population of π-electrons in hexagons. Flocke, Schmalz, and Klein[16] were first to point out to a significant and unexpected difference in the character of distinct Kekulé valence structures of C_{60} by showing that less than a half of the valence structures of buckminsterfullerene can account for about 99.82 % of molecular energy. The Atlas of Kekulé valence structures of C_{60} here compiled offers some insight into this result, which was unexpected and surprising. As one can see from the pictorial display of Kekulé valence structures given in the Appendix, the contents of Table II and Table III in the text, and the outlined classifications of Kekulé valence structures, the individual Kekulé valence structures of buckminsterfullerene differ considerably in their form, their respective patterns of CC double bonds, and consequently their relative importance to molecular energy and molecular resonance energy.

It is hoped that this Atlas may stimulate further studies on Kekulé valence structures of C_{60}. For example, as it has been suggested by one of the reviewers, the symmetry orbits of Kekulé structures span the point group representation which can be decomposed into specific irreducible representations. Such characterization of Kekulé valence structures is desirable but is far from trivial, although for some Kekulé structures it can be obtained by inspection, such as structure 1, 5, and 108.

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APPENDIX Atlas of Kekulé Valence Structures of Buckminsterfullerene

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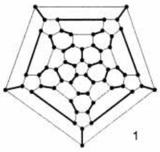

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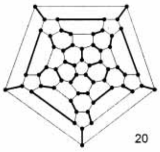

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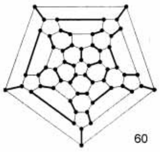

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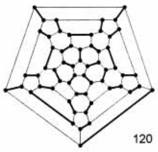

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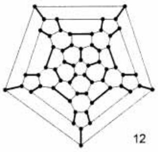

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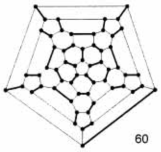

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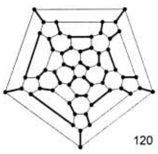

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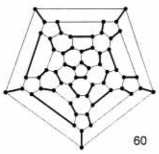

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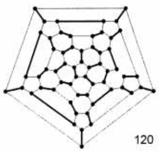

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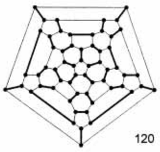

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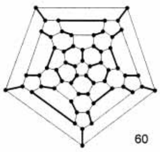

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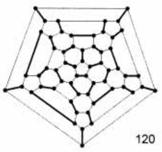

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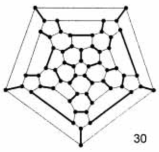

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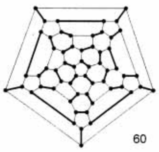

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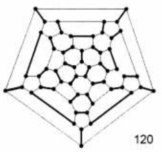

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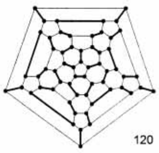

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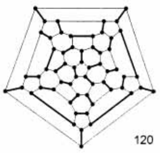

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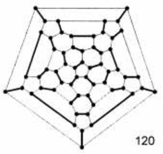

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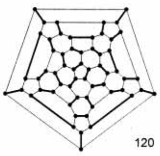

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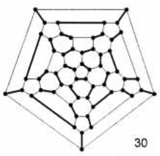

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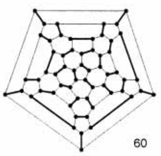

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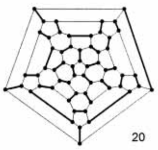

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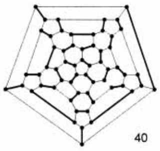

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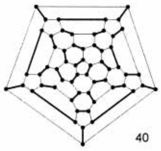

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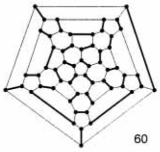

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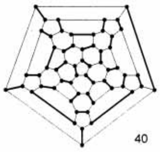

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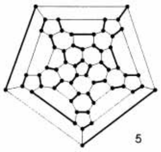

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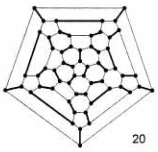

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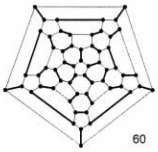

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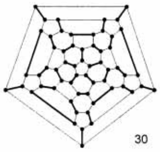

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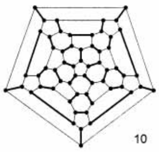

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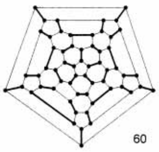

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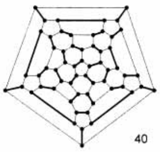

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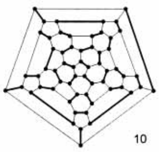

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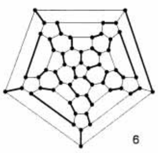

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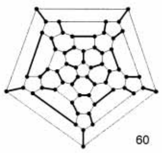

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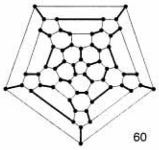

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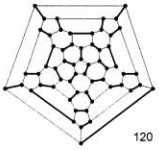

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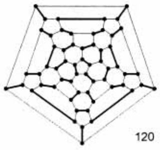

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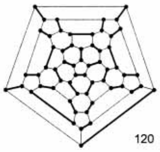

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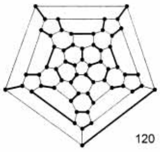

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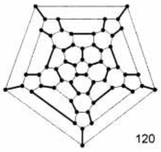

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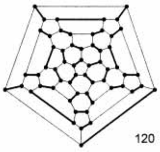

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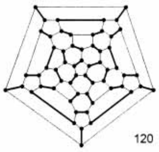

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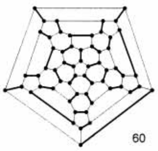

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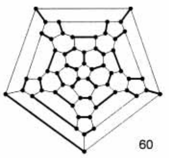

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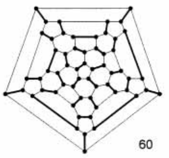

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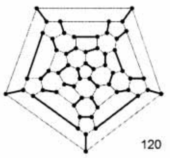

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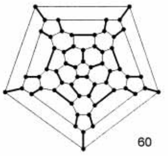

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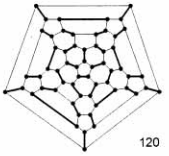

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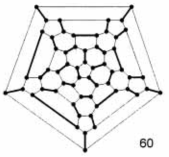

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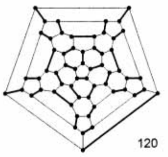

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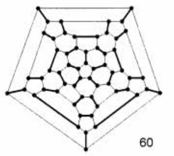

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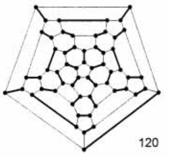

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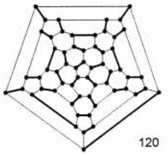

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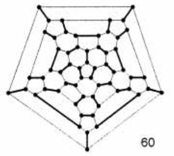

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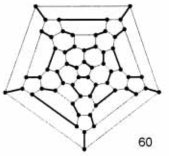

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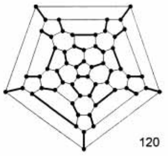

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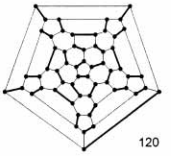

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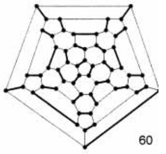

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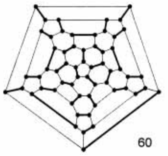

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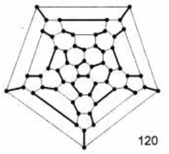

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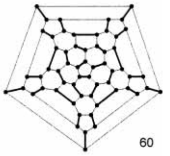

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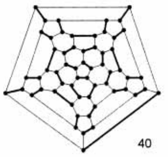

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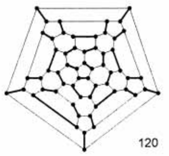

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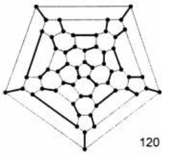

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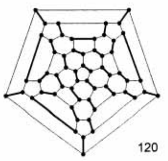

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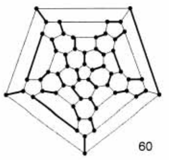

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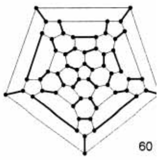

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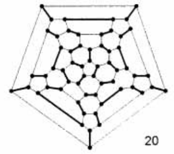

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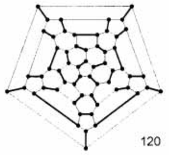

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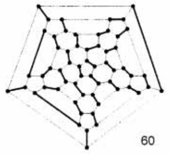

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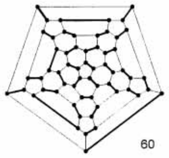

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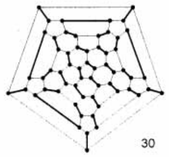

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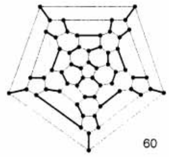

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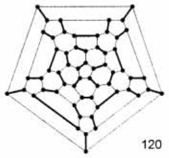

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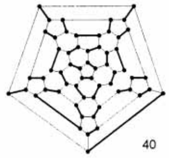

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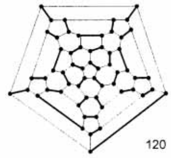

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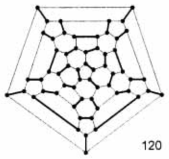

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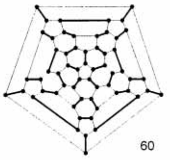

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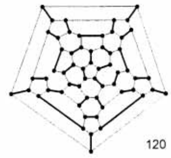

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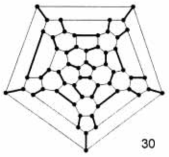

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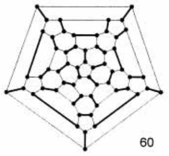

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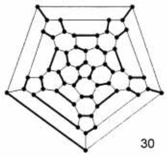

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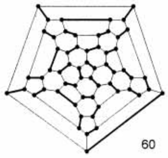

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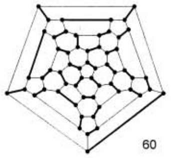

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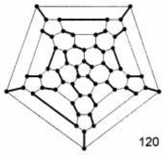

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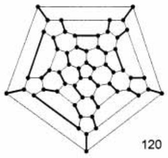

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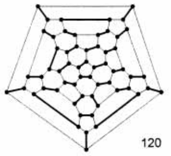

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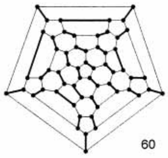

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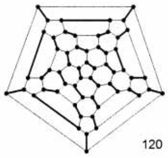

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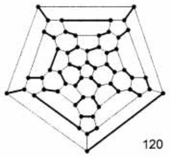

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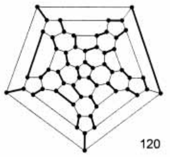

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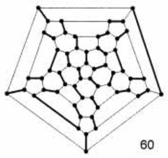

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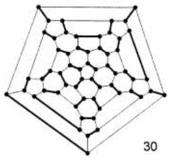

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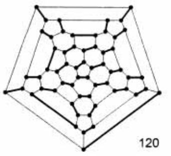

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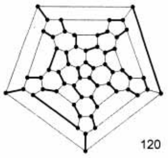

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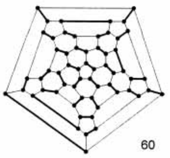

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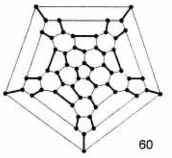

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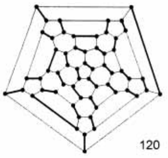

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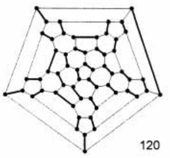

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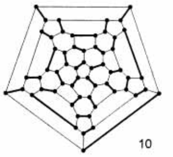

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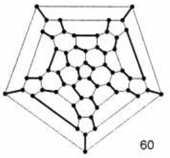

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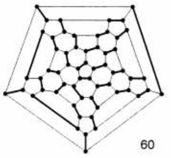

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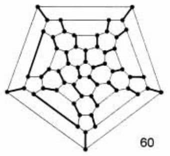

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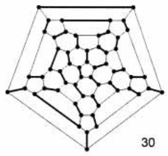

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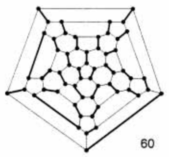

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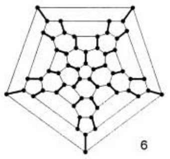

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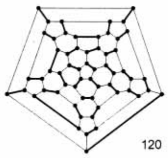

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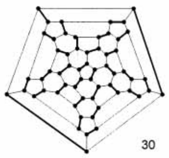

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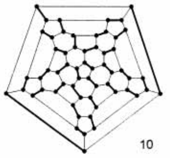

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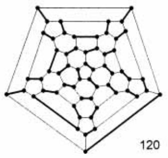

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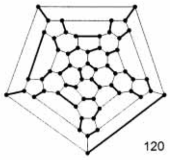

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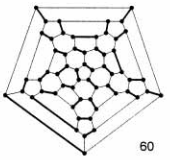

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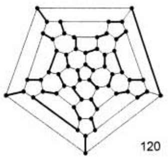

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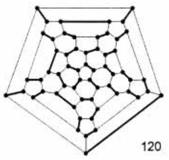

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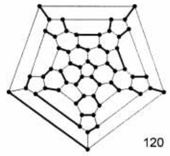

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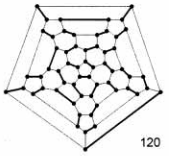

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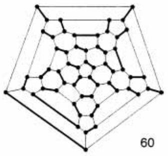

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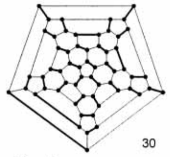

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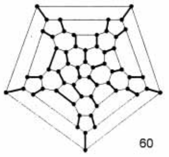

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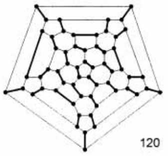

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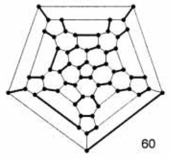

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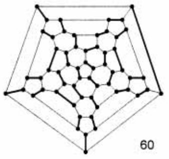

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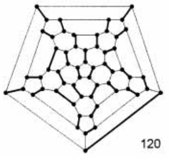

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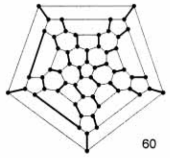

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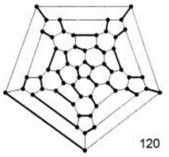

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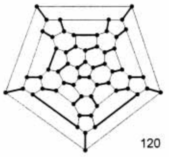

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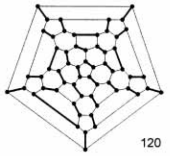

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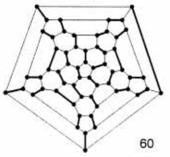

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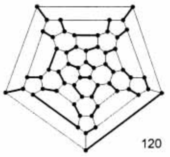

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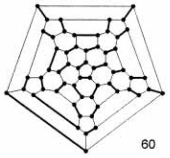

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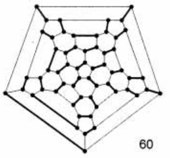

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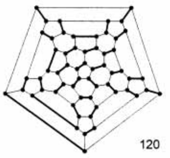

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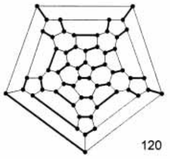

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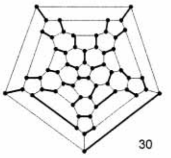

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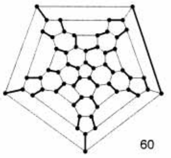

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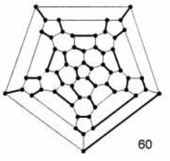

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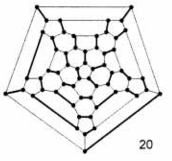

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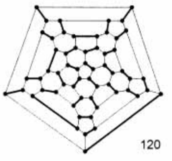

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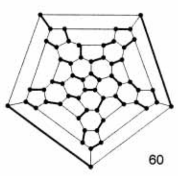

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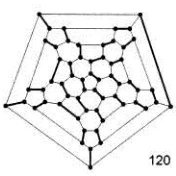

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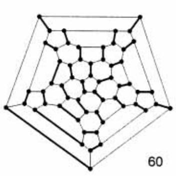

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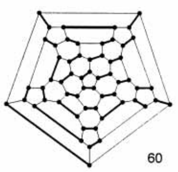

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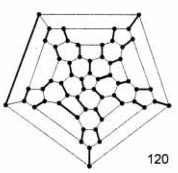

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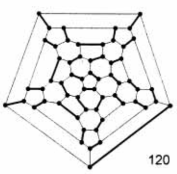

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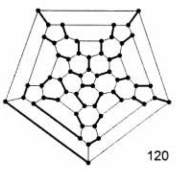

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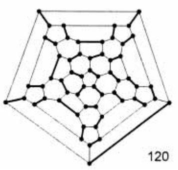

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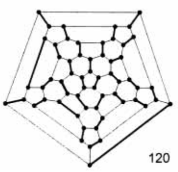

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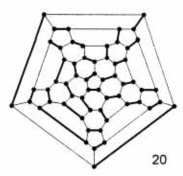

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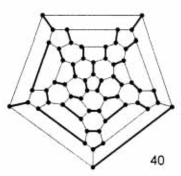

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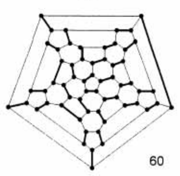

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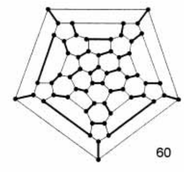

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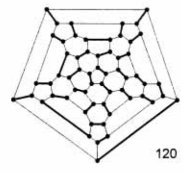

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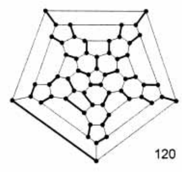

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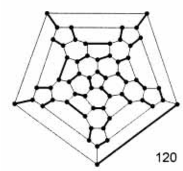

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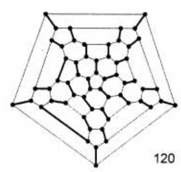

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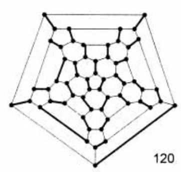

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SAŽETAK

Atlas Kekuléovih valentnih struktura Buckminsterfulerena

Damir Vukičević, Harry W. Kroto i Milan Randić

Od 12.500 Kekuléovih valentnih struktura Buckminsterfullerena samo je 158 različitih ako se razmatraju samo strukture koje su različite u odnosu na operacije simetrije. Kekuléove valentne strukture klasificirane su preme stupnju slobode (df), koji se mjenja od maksimalne vrijednosti df = 10 pa do df = 5. Najvažnija i jedinstvena Kekuléova valentna struktura u kojoj su sve CC dvostrukle veze izvan peteročlanih prstena ima stupanj slobode 10, dok broj različitih Kekuléovoh struktura obzirom na simetriju ima 36 kojim pripada stupanj slobode 5.