Kornilov M. Yu., Ljubchuk T. V., Isaev S.D., Plakhotnyk V. V., Zamkovyi V.I.

NUMBER OF ISOMERS IN ICOSAHEDRAL FULLERENE C^{60} AND Cgo SERIES

The numbers of isomers in icosahedral fullerene C^{60} and C^{g0} series have been enumerated by applying Polya's theorem and analysing symmetries of their molecular frameworks. Cycle indices have been deduced for chiral and achiral derivatives. Program operating with polydigital numbers have been applied to calculate numbers of isomeric derivatives up to C^{540}.

Buckminsterfullerene (Buckyball) C^{60} made a stir in the XX century. It was called "the most beautiful molecule" [1] and is worthy of this name. It has a nearly spherical molecule of the icosahedral point group k with 120 symmetry operations.

Buckyball has a lot of relatives that form the fullerene family. This term is assigned to carbon molecules C^n with so-called *isolated pentagon* cycles arranged between hexagons on the cage surface, which means that any couple of pentagons is separated by at least one hexagon. Buckminsterfullerene is the simplest fullerene.

Enumeration of isomers arising by addition to, or substitution in, a basic framework is a mathematical problem with many practical applications in chemistry. Therefore, it is no wonder that such a problem as applied to carbon clusters interests both chemists and mathematicians. One of the most convenient methods for solving this problem is based on Polya's and related theorems [2—10]. Thus, Balasubramanian [8—10] has enumerated the isomers of polysubstituted fullerene cages by using the cycle index of the rotational subgroup of the point group of the fullerene cage under consideration.

Other methods of isomer counting of carbon clusters have also been used. Brocas [11] has presented a systematic enumeration of dodecahedrane derivatives, which is based on double cosets and framework groups. Hflsselbarth [12] has reported an alternative method that is based on tables of marks. Mead [13] has presented an alternative method and compared above methods by using common problems.
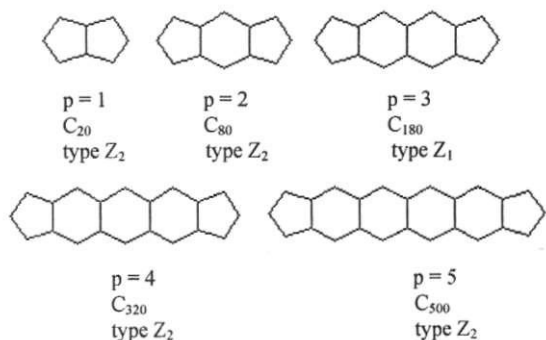
Fujita [14,15] has reported a systematic enumeration of chemical structures derived from dodecahedrane and soccerane skeletons (7/,) in terms of unit subduced cycle indices.

The classification of the simplest fullerenes based on symmetry of their molecules and isomer counting has been described for some simplest cases in [16]; the structures were confined by Ceo to C^{84} and the pencil-and-paper counting method was applied. There is no doubt automatized calculations give the results quicker and more reliable. Isomer counting in all the series presented in this paper is practically impossible without computers.

I. Vertex substitution of fullerenes

1. Some general principles of structural (position) isomers calculation.

If we consider the most symmetrical structural isomers of fullerenes with icosahedral symmetry of the group *Ih* **(IF)** we cannot avoid the yet unknown but highly possible molecule C^{20} with the dodecahedron skeleton on a purely formal basis. It has to be considered as the simplest carbon structure of *h* symmetry. In fact it is starting the **first** series of **IF**'s of the common formula $C^{20}p$, where $\rho = 1, 2, 3$, C_{20}, $C_{805}C_{180}$, C_{320}, C_{500} etc. The main structural feature of the **first** series lies in the fact that each couple of the **nearest** *pentagon* cycles is separated by p-1 hexagon cycles combined in the *linearly annelated ensembles:*
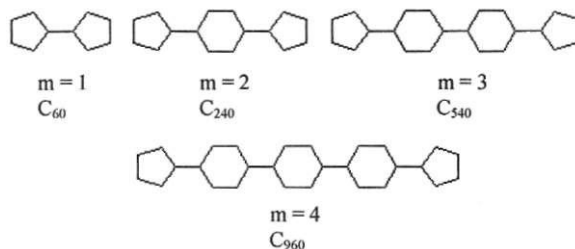

p = 1
C_{20}
type Z_2

p = 2
C_{80}
type Z_2

p = 3
C_{180}
type Z_1

p = 4
C_{320}
type Z_2

p = 5
C_{500}
type Z_2

It will be shown in the next section that the *cycle indices* of **IF** structural isomers depend on ρ values. When ρ is divisible by 3 (type Z_1. C_m, C_{720} etc.), the *cycle index* has the form (1):

$$Z_1(C_{20p^2}) = \frac{1}{120}\left(f_1^{20p^2} + 15f_1^{4p}f_2^{10p^2-2p} + 16f_2^{10p^2} + 20f_3^{\frac{20p^2}{3}} + 24f_5^{4p^2} + 20f_6^{\frac{10p^2}{3}} + 24f_{10}^{2p^2} \right) \quad (1)$$

If ρ is not divisible by 3 (type Z_2: C_{20}, C_{80}, C_{320}, C_{500}, C_{980} etc.), the *cycle index* has the form (2):

$$Z_2(C_{20p^2}) = \frac{1}{120}\left(f_1^{20p^2} + 15f_1^{4p}f_2^{10p^2-2p} + 16f_2^{10p^2} + 20f_1^2 f_3^{\frac{20p^2-2}{3}} + 24f_5^{4p^2} + 20f_2 f_6^{\frac{20p^2-2}{6}} + 24f_{10}^{2p^2} \right) \quad (2)$$

The **second** series of **IF**'s starts with the C_{60} buckminsterfullerene and has the common formula $C_{60N}A$ where $m = 1,2,3,\ldots$ (C_{60}, C_{240}, C_{540} etc.). In this series each couple of the **nearest** *pentagon* cycles is separated by p-1 hexagon cycles combined in the *para-phenylene-like ensembles:*

m = 1
C_{60}

m = 2
C_{240}

m = 3
C_{540}

m = 4
C_{960}

This kind of **IF**'s structural isomers has the cycle index (3):

$$Z_3(C_{60m^2}) = \frac{1}{120}\left(f_1^{60m^2} + 15f_1^{4m}f_2^{30m^2-2m} + 16f_2^{30m^2} + 20f_3^{20m^2} + 24f_5^{12m^2} + 20f_6^{10m^2} + 24f_{10}^{6m^2} \right) \quad (3)$$

The numbers of isomers formed by adding one or more couples of hydrogens or other atoms to the fullerene skeleton (for example, $C_{60}H_2$ or $C_{60}Cl_4$), substituting heteroatoms for carbons (for example, $C_{79}Si$ or $C_{78}N_2^{2+}$) or substituting other atoms or groups for hydrogens in fully hydrogenated fullerenes (for example, $C_{60}H_{58}Cl_2$), can be calculated by the standard substitution of $(1+x^m)^n$ for *fl* into the formulae {Yy-(3), which gives the *generating functions*. Here is the beginning of the generating functions for C_{60} and C_{80}:

$$P(C_{60}) = \sum_0^N a_i x^i = 1 + x + 23x^2 + 303x^3 + 4190x^4 + 45718x^5 + 418470x^6 + 3220218x^7 + \ldots$$

$$P(C_{80}) = \sum_0^N a_i x^i = 1 + 2x + 40x^2 + 732x^3 + 13506x^4 + 201230x^5 + 2508958x^6 + 26484548x^7 + \ldots$$

The coefficients a_i of above generating functions correspond to the numbers of structural isomers of fullerene addition-products or their heteroanalogues. For example, there may be 2 theoretically possible structural isomers of $C_{79}Si$, 40 dications $C_{78}N_2^{2+}$, 732 trications $C_{77}N_3^{3+}$, 23 structural isomers of $C_{60}H_2$, 4190 isomers of $C_{60}Cl_4$ or 303 isomers of $C_{60}H_{57}Cl_3$. The coefficients a_j were calculated with the help of a special

program operating with large polydigital numbers. **It** is obvious that the pencil-and-paper method would not work here.

If we need to calculate the numbers of isomers for the cases of different substituents or different heteroatoms we have to substitute $(1 + x^m + y^m + \dots)^n$ for $/,,"$ in the *cycle indices* formulae (1) — (5). It is not so simple a procedure as to use the pencil-and-paper method but the computer program works here too.

2. Stereoisomerism of fullerenes.

Until now we had not taken into account the stereoisomerism of fullerenes. Actually, some of structural isomers are chiral, others are not. The total number S^n of stereoisomers includes Q^n couples of chiral and R^n achiral structures, i.e. $S^n = 2Q^n + R^n$, while the number of structural isomers that do not take into account the **IF**'s stereoisomerism, is $P^0 = Q^n + R^n$. Thus, $Q^n = S^n - P^n$. It may be shown that chirality is the reflection of the corresponding molecular polygon symmetry. The **IF**'s stereoisomers produce a symmetry group of rotations $/$ that has half as many symmetry operations (60) as the **IF**'s structural isomers with their group Ih (120 symmetry operations). The corresponding *cycle indices* are the following:

$$Z_4(C_n) = \frac{1}{60}\left(f_1^n + 15f_2^{\frac{n}{2}} + 20f_3^{\frac{n}{3}} + 24f_5^{\frac{n}{5}}\right), \qquad (4)$$

if η is divisible by 3, and

$$Z_5(C_n) = \frac{1}{60}\left(f_1^n + 15f_2^{\frac{n}{2}} + 20f_1^2 f_3^{\frac{n-2}{3}} + 24f_5^{\frac{n}{5}}\right), \qquad (5)$$

if n is not divisible by 3.

II. Edge substitution of fullerenes

As it has been above shown (see 1.1) there are two series of structural isomers of **IF**'s with the common formulae $C_{2o_p}2$ and $C_{6o_m}2$. Their cycle indices of edge substitution are following:

$$Z_6(C_{20p^2}) = \frac{1}{120}\left(f_1^{30p^2} + f_2^{15p^2} + 15f_1^{4p} f_2^{15p^2-2p} + \right.$$
$$+15f_1^2 f_2^{15p^2-1} + 20f_3^{10p^2} + 24f_5^{6p^2} +$$
$$\left. + 20f_6^{5p^2} + 24f_{10}^{3p^2}\right)$$

and

$$Z_7(C_{60m^2}) = \frac{1}{120}\left(f_1^{90m^2} + f_2^{45m^2} + 15f_1^{8m} f_2^{45m^2-4m} + \right.$$
$$+15f_1^2 f_2^{45m^2-1} + 20f_3^{30m^2} + 24f_5^{18m^2} +$$
$$\left. + 20f_6^{15m^2} + 24f_{10}^{9m^2}\right).$$

The cycle indices for stereoisomers of IF's take the form:

$$Z_8(C_n) = \frac{1}{60}\left(f_1^e + 15f_1^2 f_2^{\frac{e-2}{2}} + 20f_3^{\frac{e}{3}} + 24f_5^{\frac{e}{5}}\right),$$

where *e* is the number of edges in the fullerene.
Edge substitution of fullerenes takes place when

oxygen or methylene group bridges an edge, or in hypothetical expanded cages where a fullerene C—C edge becomes C—C=C—C linkage [17] etc. Addition reactions of fullerenes, for example, the reduction through hydrogenation can also be considered as edge substitution as by the reaction double bonds transform into single ones. As attachment occurs only at formal double bonds of fullerenes, the corresponding modified cycle indices of IF structural isomers assume the form:

$$Z_6'(C_{20p^2}) = \frac{1}{120}\left(f_1^{10p^2} + f_2^{5p^2} + 15f_1^{4p-4} f_2^{5p^2-2p+2} + \right.$$
$$+15f_1^2 f_2^{5p^2-1} + 20f_3^{\frac{10p^2}{3}} + 24f_5^{2p^2} +$$
$$\left. + 20f_6^{\frac{10p^2}{6}} + 24f_{10}^{p^2}\right),$$

if ρ is divisible by 3;

$$Z_7'(C_{60m^2}) = \frac{1}{120}\left(f_1^{30m^2} + f_2^{15m^2} + 15f_1^{4m} f_2^{15m^2-2m} + \right.$$
$$+15f_1^2 f_2^{15m^2-1} + 20f_3^{10m^2} + 24f_5^{6m^2} +$$
$$\left. + 20f_6^{5m^2} + 24f_{10}^{3m^2}\right).$$

If only double bonds are taken into account, the cycle indices for stereoisomers of IF's depend on ρ value (here *d* is the number of double bonds):

$$Z_8'(C_n) = \frac{1}{60}\left(f_1^d + 15f_1^2 f_2^{\frac{d-2}{2}} + 20f_3^{\frac{d}{3}} + 24f_5^{\frac{d}{5}}\right),$$

when ρ is divisible by 3.

In case C_{20p2} of fullerenes where ρ is not divisible by 3 introduction of formal double bonds reduces the symmetry of structures, and their cycle indices of edge substitution for double bonds will be not here considered.

III. The action of a group of symmetries I_h and a group of rotations $/$ on a set of fullerene vertices

The Ih symmetry group is a symmetry group of fullerenes C_n (n is the number of carbon atoms) at the uniform distribution of 5-faces on the fullerene surface. This is the case when $\eta = 60m^2$ or $\eta = 20p^2$, where m, ρ are natural numbers. The h group has the $/$ icosahedral subgroup of rotations of order 60.

Here is a pel-by-pel description of the elements of above groups (see also Table 1).

1. The neutral element of Д and $/$ groups does not move any vertex; it is a product of η cycles of length 1.

2. Inversion which is an element of I_h group reflects each fullerene vertex into its diametrically opposite one. The inversion is a product of n/2 cycles of length 2.

3. Each of 15 rotations by the angle 180° defines the symmetry axis that passes through the middles of the opposite edges; 15 corresponding elements of Д or $/$ groups are products of n/2 cycles of length 2.

4. Each of 24 rotations by angles divisible by 72° defines in their totality 6 axes of rotations by these angles which pass through centres of the opposite fullerene 5-faces; each of 24 corresponding elements of Д or / groups is a product of n/5 cycles of length 5.

5. Each of 20 rotations by the angles divisible by 120° defines in their totality 10 axes of rotations by these angles which pass through a couple of diametrically opposite points — centres of triangles the vertices of which are centres of the nearest fullerene 5-faces; each of 20 corresponding elements of //, and / groups are products of n/3 cycles of length 3 in case $\eta = 60m^2$ or $\eta = 20p^2$, where ρ is divisible by 3. It is a product of two cycles of length 1 and (n-2)/3 cycles of length 3 in case $\eta = 20p^2$, where ρ is not divisible by 3.

6. Each of 15 symmetry operations relative to the plane reflects each of fullerene vertices into the symmetrical one relative to the plane, each plane passing through 4m fullerene vertices when $\eta = 60m^2$ and through 4p fullerene vertices when $\eta = 20p^2$. Each of 15 corresponding elements of I_h group is a product of 4m cycles of length 1 and $30m^2 - 2m$ cycles of length 2 in case $\eta = 60m^2$ or 4p cycles of length 1 and $10p^2 - 2p$ cycles of length 2 in case $\eta = 20p^2$.

7. Each of 24 mirror rotations by angles divisible by 72° is a consecutive execution of the inversion and rotation described above; elements of I_h group are products of n/10 cycles of length 10.

8. Each of 20 mirror rotations by angles divisible by 120° is a consecutive execution of the inversion and rotation described above; each of 20 corresponding elements of Ih group is a product of n/6 cycles of length 6 in case $\eta = 60m^2$ or $\eta = 20p^2$, where ρ is divisible by 3 and is a product of two cycles of length 2 and (n-2)/6 cycles of length 6 in case $\eta = 20p^2$, when ρ is not divisible by 3.

Summary

The isomer numbers of fullerenes can be calculated on the basis of cycle indices of their molecular frameworks. The cycle indices result from the analysing frameworks symmetries. Cycle indices of vertex and edge substitution for fullerenes of Ih symmetry have been developed and generalized. It has been shown that there are two series of structural isomers of fullerenes with the common formulae C_{20p2} and C_{60m2} which form icosahedral I_h symmetry group. The stereoisomers of fullerenes belong to icosahedral I subgroup. The standard transformation of the cycle indices into generating functions results in the values of structural isomers or stereoisomers of fullerenes. Chiral and achiral derivatives have been counted separately.

Table 1. **The terms in the cycle indices.**

The item	Z_1	Z_2	Z_3	Z_4	Z_5	Z_6	Z_7	Z_8
1	$f_1^{20p^2}$	$f_1^{20p^2}$	$f_1^{60m^2}$	f_1^n	f_1^n	$f_1^{30p^2}$	$f_1^{90m^2}$	f_1^e
2	$f_2^{10p^2}$	$f_2^{10p^2}$	$f_2^{30m^2}$	—	—	$f_2^{15p^2}$	$f_2^{45m^2}$	—
3	$15f_2^{10p^2}$	$15f_2^{10p^2}$	$15f_2^{30m^2}$	$15f_2^{\frac{n}{2}}$	$15f_2^{\frac{n}{2}}$	$15f_1^2 f_2^{15p^2-1}$	$15f_1^2 f_2^{45m^2-1}$	$15f_1^2 f_2^{\frac{e-2}{2}}$
4	$24f_5^{4p^2}$	$24f_5^{4p^2}$	$24f_5^{12m^2}$	$24f_5^{\frac{n}{5}}$	$24f_5^{\frac{n}{5}}$	$24f_5^{6p^2}$	$24f_5^{18m^2}$	$24f_5^{\frac{e}{5}}$
5	$20f_3^{\frac{20p^2}{3}}$	$20f_1^2 f_3^{\frac{20p^2-2}{3}}$	$20f_3^{20m^2}$	$20f_3^{\frac{n}{3}}$	$20f_1^2 f_3^{\frac{n-2}{3}}$	$20f_3^{10p^2}$	$20f_3^{30m^2}$	$20f_3^{\frac{e}{3}}$
6	$15f_1^{4p} f_2^{10p^2-2p}$	$15f_1^{4p} f_2^{10p^2-2p}$	$15f_1^{4m} f_2^{30m^2-2m}$	—	—	$15f_1^{4p} f_2^{15p^2-2p}$	$15f_1^{8m} f_2^{45m^2-4m}$	—
7	$24f_{10}^{2p^2}$	$24f_{10}^{2p^2}$	$24f_{10}^{6m^2}$	—	—	$24f_{10}^{3p^2}$	$24f_{10}^{9m^2}$	—
8	$20f_6^{\frac{10p^2}{3}}$	$20f_2 f_6^{\frac{20p^2-2}{6}}$	$20f_6^{10m^2}$	—	—	$20f_6^{5p^2}$	$20f_6^{15m^2}$	—

Table 2. **Buckminsterfullerene C_{60} and its isomers of vertex substitution**
(N — the number of substituents).

N	stereoisomers (chiral and achiral isomers)	structural (position) isomers	chiral isomers (enantiomer pairs)	achiral isomers
0	1	1	0	1
1	1	1	0	1
2	37	23	14	9
3	577	303	274	29
4	8236	4190	4046	144
5	91030	45718	45312	406
6	835476	418470	417006	1464

N	stereoisomers (chiral and achiral isomers)	structural (position) isomers	chiral isomers (enantiomer pairs)	achiral isomers
7	6436782	3220218	3216564	3654
8	42650532	21330558	21319974	10584
9	246386091	123204921	123181170	23751
10	1256602779	628330629	628272150	58479
11	5711668755	2855893755	2855775000	118755
12	23322797475	11661527055	11661270420	256635
13	86114390460	43057432740	43056957720	475020
14	289098819780	144549869700	144548950080	919620
15	886568158468	443284859624	443283298844	1560780
16	2493474394140	1246738569480	1246735824660	2744820
17	6453694644705	3226849468425	3226845176280	4292145
18	15417163018725	7708584971055	7708578047670	6923385
19	34080036632565	17040023323785	17040013308780	10015005
20	69864082608210	34932048763560	34932033844650	14918910
21	133074428781570	66537224405790	66537204375780	20030010
22	235904682814710	117952355252550	117952327562160	27690390
23	389755540347810	194877787472550	194877752875260	34597290
24	600873146368170	300436595453640	300436550914530	44539110
25	865257299572455	432628675734195	432628623838260	51895935
26	1164769471671687	582384767014701	582384704656986	62357715
27	1466746704458899	733373386161407	733373318297492	67863915
28	1728665795116244	864332935668892	864332859447352	76221540
29	1907493251046152	953746664302456	953746586743696	77558760
30	1971076398255692	985538239868528	985538158387164	81481364

Table 3. **C$_{80}$ and its isomers of vertex substitution (N — the number of substituents).**

N	stereoisomers (chiral and achiral isomers)	structural (position) isomers	chiral isomers (enantiomer pairs)	achiral isomers
0	1	1	0	1
1	2	2	0	2
2	63	40	23	17
3	1378	732	646	86
4	26572	13506	13066	440
5	400682	201230	199452	1778
6	5010915	2508958	2501957	7001
7	52945490	26484548	26460942	23606
8	483148575	241613043	241535532	77511
9	3865005820	1932616241	1932389579	226662
10	27441701452	13721174187	13720527265	646922
11	174627951940	87314815907	87313136033	1679874
12	1004111683250	502057977058	502053706192	4270866
13	5252271461480	2626140736951	2626130724529	10012422
14	25135875183830	12567949113763	12567926070067	23043696
15	110597830301160	55298939830653	55298890470507	49360146
16	449303704778500	224651904399560	224651800378940	104020620
17	1691496227818540	845748216614906	845748011203634	205411272
8	5920236865724610	2960118632726706	2960118232997904	399728802

N	stereoisomers (chiral and achiral isomers)	structural (position) isomers	chiral isomers (enantiomer pairs)	achiral isomers
19	19318667443935860	9659334088315142	9659333355620718	732694424
20	58921935915528842	29460968620341478	29460967295187364	1325154114
21	168348387724608520	84174194995664136	84174192728944384	2266719752
22	451479767657432800	225739885743444420	225739881913988380	3829456040
23	1138514195243025640	569257100690889408	569257094552136232	6138753176
24	2703971215098899265	1351985612412704125	1351985602686195140	9726508985
25	6056895518692773170	3028447766677152629	3028447752015620541	14661532088
26	12812663600241332049	6406331811049131897	6406331789192200152	21856931745
27	25625327194466052658	12812663612765383757	12812663581700668901	31064714856
28	48505083623898300868	24252541833791614034	24252541790106686834	43684927200
29	86974632694515291154	43487316376592019173	43487316317923271981	58668747192
30	147856875590732334429	73928437834359788281	73928437756372546148	77987242133
31	238478831581736161130	119239415840437268425	119239415741298892705	99138375720
32	365170710875242870325	182585355500008169677	182585355375234700648	124773469029
33	531157397613861592600	265578698882098856330	265578698731762736270	150336120060
34	734246990841346298680	367123495510359861590	367123495330986437090	179373424500
35	965010330790896021320	482505165497972227150	482505165292923794170	205048432980
36	1206262913516965086380	603131456874559086076	603131456642406000304	232153085772
37	1434474816040523716160	717237408146242476910	717237407894281239250	251961237660
38	1623221502394461793460	811610751332664213166	811610751061797580294	270866632872
39	1748084694850998206080	874042347565112895050	874042347285885311030	279227584020
40	1791786812256738178780	895893406270934688580	895893405985803490200	285131198380

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Корнілов М.Ю., Любчук Т.В., Ісаєв С.Д., Плахотнік В.В., Замковий В.І.

КІЛЬКІСТЬ ІЗОМЕРІВ В ІКОСОЕДРАЛЬНИХ ФУЛЕРЕНАХ СЕРІЙ C⁶⁰ ТА C⁸⁰

Використовуючи теорему Пойя та аналізуючи симетрію фрагментів, обчислено кількість ізомерів в ікосоедральних фулеренах серій $C^{в0}$ та C^{80}. Виведені циклові індекси для хіральних та ахіральних похідних. Для обчислення кількості ізомерів фулеренів до C^{540} використана програма маніпуляції з багатознаковими числами.