The Cycle Index of the Symmetry Group of the Fullerene C_{60}

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Abstract

Various forms, including multi-dimensional forms of the cycle index of the symmetry group of the fullerene C_{60} acting on its sets of vertices, faces, edges etc. are computed and applied for the enumeration of *essentially different* colourings of the truncated icosahedron. The implementation of these cycle index methods in the computer algebra system SYMMETRICA is discussed, and finally cycle indices of the symmetry groups of some further fullerenes are derived.

1 Introduction

In 1985 the first C_{60} clusters were produced and it was assumed [21] that its 60 carbon atoms are placed at the vertices of a *truncated icosahedron* (which is commonly called a *foot ball* or *soccer ball*.) The truncated icosahedron is one of the 14 *Archimedean solids* already known to the ancient Greeks. Five years later [20, 24] the original hypotheses on the structure of C_{60} could be confirmed. A nice introduction into the theory of the fullerenes providing historical and chemical background information can be found in [10]. From the mathematical point of view in the present paper we are interested in the combinatorics of the symmetry group of the truncated icosahedron and we will discuss some examples in how many ways the soccer ball can be coloured in *essentially different* ways. From the chemical point of view we will determine the number of all possible placements of double bonds for the C_{60} fullerene. Furthermore investigating the $C_{60}H_{60}$-molecule (i.e. a hypothetic molecule where all the thirty double bonds of the C_{60} are hydrated), we will compute the numbers of all $C_{60}H_kCl_{60-k}$ molecules. Finally the implementation of these cycle index methods in the computer algebra system SYMMETRICA [23] will be discussed and some further cycle indices will be listed.

2 Some cycle indices

For applying Pólya theory to the combinatorics of the fullerene C_{60} we must determine the *cycle index* of the *symmetry group* of the truncated icosahedron. Let G be a multiplicative group and let X be a set then a *group action* of G on X is given by a mapping

$$G \times X \to X, \qquad (g, x) \mapsto g \cdot x,$$

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such that $g_1 \cdot (g_2 \cdot x) = (g_1 g_2) \cdot x$ and $1 \cdot x = x$ for all $g_1, g_2 \in G$ and $x \in X$. The *orbit* of $x \in X$ is the set $G(x) := \{g \cdot x \mid g \in G\}$. The cycle index of a finite group G acting on a finite set X is a polynomial in indeterminates $x_1, x_2, \ldots$ over the set of rationals given by

$$Z(G, X) := \frac{1}{|G|} \sum_{g \in G} \prod_{i=1}^{|X|} x_i^{a_i(\bar{g})},$$

where $\bar{g}$ is the *permutation representation* of g and $(a_1(\bar{g}), \ldots, a_{|X|}(\bar{g}))$ is the *cycle type* of the permutation $\bar{g}$. For more details about cycle indices (and about combinatorics via finite group actions in general) see [18].

From the way of constructing the truncated icosahedron from the *icosahedron* (see figure 1) it is clear that they both have the same symmetry group $\mathcal{S}$ which is isomorphic to $A_5 \times S_2$. The *rotational symmetries* form a subgroup $\mathcal{R}$ of $\mathcal{S}$ of index 2 which is isomorphic to A_5. The point group symbols for $\mathcal{S}$ and $\mathcal{R}$ are $\mathrm{I_h}$ and I.

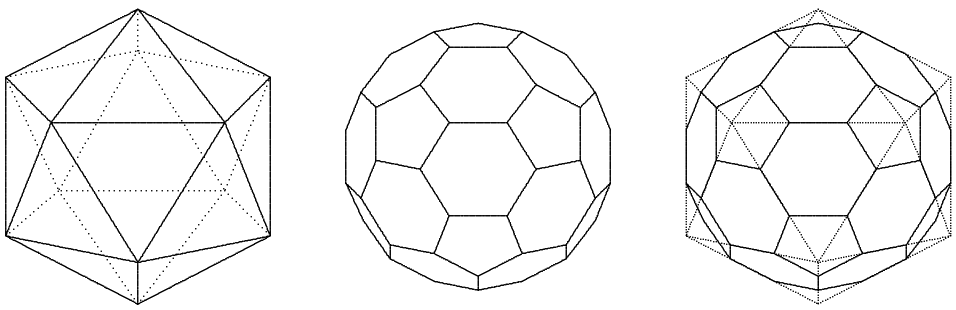

Figure 1: The icosahedron and the C_{60}-fullerene

The elements of $\mathcal{R}$ can be described in the following way: The 12 pentagonal faces of the fullerene C_{60} form 6 pairs of opposite faces. A rotation axis through the centres of two such faces is an axis of a 5-fold rotation. The 20 hexagonal faces of the fullerene C_{60} form 10 pairs of opposite faces through the centres of which we each have an axis of a 3-fold rotation. Finally the set of edges can be partitioned into 60 *pentagonal edges* surrounding the pentagonal faces and 30 *hexagonal edges* lying between two hexagons. The hexagonal edges form 15 pairs of opposite edges the centres of which each determine an axis of a 2-fold rotation. The full symmetry group of the fullerene C_{60} is computed by combining these rotations with one reflection of the fullerene.

In the present paper the symmetries of a fullerene are described as permutations of its set of vertices. This permutation representation induces a group action on the sets of all edges or faces by identifying an edge or a face with the vertices incident to it. The generators of $\mathcal{R}$ will be indicated by π_1 and π_2, whereas σ stands for a reflection.

Labelling the vertices of the fullerene C_{60} as is indicated in figure 2 the permutation representation of generators of $\mathcal{R}$ and $\mathcal{S}$ acting on the set of vertices is given by:

$\pi_1 =$ (56,57,58,59,60)(51,52,53,54,55)(42,44,46,48,50)(41,43,45,47,49)(32,34,36,38,40)
(31,33,35,37,39)(22,24,26,28,30)(21,23,25,27,29)(12,14,16,18,20)(11,13,15,17,19)
(6,7,8,9,10)(1,2,3,4,5)

$\pi_2 =$ (37,38,48,54,47)(27,28,49,59,46)(18,39,60,53,26)(17,29,55,58,36)(10,40,56,45,16)(9,19,50,57,35)(7,12,22,23,13)(5,30,51,44,15)(4,20,41,52,25)(3,6,31,43,24)(2,11,32,33,14)(1,21,42,34,8)

$\sigma =$ (58)(57,59)(56,60)(53)(52,54)(51,55)(45,46)(44,47)(43,48)(42,49)(41,50)(35,36)(34,37)(33,38)(32,39)(31,40)(25,26)(24,27)(23,28)(22,29)(21,30)(15,16)(14,17)(13,18)(12,19)(11,20)(8,9)(7,10)(6)(3,4)(2,5)(1)

π_1 is a 5-fold rotation around the centre of figure 2 and π_2 is a 5-fold rotation, where the rotation axis goes through the centres of the faces $\{7, 12, 22, 23, 13\}$ and $\{37, 38, 48, 54, 47\}$.

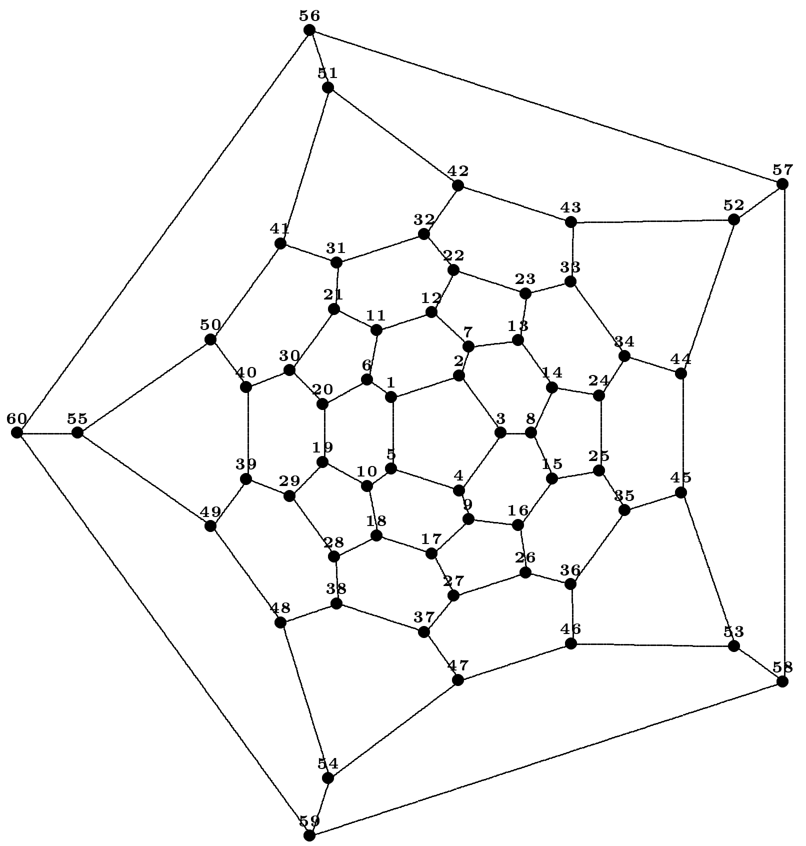

Figure 2: Labelling the vertices of the fullerene C_{60}, given by its Schlegel diagram

There are computer algebra systems which evaluate the cycle index of a permutation group given by a set of generators. For instance the SYMMETRICA routine `zykelind_arb(a,b)` computes the cycle index `b` of a permutation group with generators given in the `VECTOR`-object `a`. In this way the cycle indices of $\mathcal{R}$ and $\mathcal{S}$ acting on the set of vertices are computed as

$$Z(\mathcal{R}, \text{Vertices}) = \frac{1}{60}(24x_5^{12} + 20x_3^{20} + 15x_2^{30} + x_1^{60})$$

$$Z(\mathcal{S}, \text{Vertices}) = \frac{1}{120}(24x_{10}^{6} + 20x_6^{10} + 24x_5^{12} + 20x_3^{20} + 16x_2^{30} + 15x_1^4x_2^{28} + x_1^{60}).$$

When labelling the edges of the fullerene C_{60} as is indicated in table 1 the generators of the induced permutation group on the set of edges of the fullerene are given by:

$\pi_1 =$ (86,87,88,89,90)(81,82,83,84,85)(72,74,76,78,80)(71,73,75,77,79)(58,61,64,67,70)(57,60,63,66,69)(56,59,62,65,68)(43,46,49,52,55)(42,45,48,51,54)(41,44,47,50,53)

(36,37,38,39,40)(27,29,31,33,35)(26,28,30,32,34)(13,16,19,22,25)(12,15,18,21,24)
(11,14,17,20,23)(6,7,8,9,10)(1,2,3,4,5)
$\pi_2 =$ (51,67,78,77,66)(50,52,68,84,65)(33,69,90,76,39)(32,40,79,89,64)(22,54,86,75,31)
(21,53,85,83,49)(20,34,80,88,48)(19,23,70,87,63)(13,27,37,28,14)(10,55,81,62,18)
(9,24,56,82,47)(7,12,43,44,15)(6,41,59,46,8)(5,36,72 ,61,17)(4,35,71,74,30)
(3,25,57,73,38)(2,11,42,60,29)(1,26,58,45,16)
$\sigma =$ (88,89)(87,90)(86)(83)(82,84)(81,85)(75,76)(74,77)(73,78)(72,79)(71,80)(63,64)
(62,65)(61,66)(60,67)(59,68)(58,69)(57,70)(56)(48)(47,49)(46,50)(45,51)(44,52)(43,53)
(42,54)(41,55)(38,39)(37,40)(36)(30,31)(29,32)(28,33)(27,34)(26,35)(18)(17,19)(16,20)
(15,21)(14,22)(13,23)(12,24)(11,25)(8,9)(7,10)(6)(3)(2,4)(1,5)
The cycle indices for the corresponding actions on the set of edges are given as

$$Z(\mathcal{R}, \text{Edges}) = \frac{1}{60}(24x_5^{18} + 20x_3^{30} + 15x_1^2x_2^{44} + x_1^{90})$$

$$Z(\mathcal{S}, \text{Edges}) = \frac{1}{120}(24x_{10}^9 + 20x_6^{15} + 24x_5^{18} + 20x_3^{30} + x_2^{45} + 15x_1^2x_2^{44} + 15x_1^8x_2^{41} + x_1^{90}).$$

Finally for the action on the set of all faces we have

$$Z(\mathcal{R}, \text{Faces}) = \frac{1}{60}(15x_2^{16} + 24x_1^2x_5^6 + 20x_1^2x_3^{10} + x_1^{32})$$

$$Z(\mathcal{S}, \text{Faces}) = \frac{1}{120}(24x_2x_{10}^3 + 20x_2x_6^5 + 16x_2^{16} + 24x_1^2x_5^6 + 20x_1^2x_3^{10} + 15x_1^8x_2^{12} + x_1^{32}).$$

Edge	Nr.	Edge	Nr.	Edge	Nr.	Edge	Nr.	Edge	Nr.
$\{1,2\}$	1	$\{9,16\}$	19	$\{22,23\}$	37	$\{30,40\}$	55	$\{43,52\}$	73
$\{2,3\}$	2	$\{9,17\}$	20	$\{24,25\}$	38	$\{41,50\}$	56	$\{44,52\}$	74
$\{3,4\}$	3	$\{17,18\}$	21	$\{26,27\}$	39	$\{31,41\}$	57	$\{45,53\}$	75
$\{4,5\}$	4	$\{10,18\}$	22	$\{28,29\}$	40	$\{32,42\}$	58	$\{46,53\}$	76
$\{1,5\}$	5	$\{10,19\}$	23	$\{21,31\}$	41	$\{42,43\}$	59	$\{47,54\}$	77
$\{1,6\}$	6	$\{19,20\}$	24	$\{31,32\}$	42	$\{33,43\}$	60	$\{48,54\}$	78
$\{2,7\}$	7	$\{6,20\}$	25	$\{22,32\}$	43	$\{34,44\}$	61	$\{49,55\}$	79
$\{3,8\}$	8	$\{11,21\}$	26	$\{23,33\}$	44	$\{44,45\}$	62	$\{50,55\}$	80
$\{4,9\}$	9	$\{12,22\}$	27	$\{33,34\}$	45	$\{35,45\}$	63	$\{51,56\}$	81
$\{5,10\}$	10	$\{13,23\}$	28	$\{24,34\}$	46	$\{36,46\}$	64	$\{52,57\}$	82
$\{6,11\}$	11	$\{14,24\}$	29	$\{25,35\}$	47	$\{46,47\}$	65	$\{53,58\}$	83
$\{11,12\}$	12	$\{15,25\}$	30	$\{35,36\}$	48	$\{37,47\}$	66	$\{54,59\}$	84
$\{7,12\}$	13	$\{16,26\}$	31	$\{26,36\}$	49	$\{38,48\}$	67	$\{55,60\}$	85
$\{7,13\}$	14	$\{17,27\}$	32	$\{27,37\}$	50	$\{48,49\}$	68	$\{56,60\}$	86
$\{13,14\}$	15	$\{18,28\}$	33	$\{37,38\}$	51	$\{39,49\}$	69	$\{56,57\}$	87
$\{8,14\}$	16	$\{19,29\}$	34	$\{28,38\}$	52	$\{40,50\}$	70	$\{57,58\}$	88
$\{8,15\}$	17	$\{20,30\}$	35	$\{29,39\}$	53	$\{41,51\}$	71	$\{58,59\}$	89
$\{15,16\}$	18	$\{21,30\}$	36	$\{39,40\}$	54	$\{42,51\}$	72	$\{59,60\}$	90

Table 1: Labelling of the edges of the fullerene C_{60}

	$\mathcal{R}$	$\mathcal{S}$
Vertices	19 215 358 678 900 736	9 607 679 885 269 312
Edges	20 632 333 988 107 263 792 381 952	10 316 166 994 124 293 843 474 944
Faces	71 600 640	35 931 952

Table 2: Different colourings of the fullerene C_{60} with 2 colours

3 Some counting problems

In his invited lecture *"Chemical Isomerism, a Challenge for Algebraic Combinatorics and for Computer Science"* at the AAECC-11 A. Kerber [8] said:

> [...] The existence of chemical isomerism was stated by the end of the eighteenth century, it was verified a quarter of a century later and explained another half of a century afterwards. It stimulated the development of graph theory and gave birth to algebraic combinatorics. [...]

The most famous starting point for enumeration under group action is [22] in which Pólya not only describes cycle index techniques for determining the numbers of orbits under finite group actions, but he demonstrates how to apply these methods for the chemical problem of isomer enumeration as well.

A colouring of the vertices, edges or faces of a fullerene with k colours can be interpreted as a function from the set of all vertices, edges or faces into the set of k colours. Two colourings are called *different* if and only if the corresponding functions lie in different orbits of the group $\mathcal{R}$ or $\mathcal{S}$ acting on the set of all these functions in a natural way. This means that the group is acting on the domain of these functions. From the cycle indices above you can compute the number of *different* colourings using k colours via Pólya-theory by replacing each variable x_i in the cycle index by k. In SYMMETRICA there is the routine `polya_const_sub(a,b,c)` which does this substitution. `a` is the cycle index, `b` takes the constant k and `c` is the result. The numbers of *different* colourings with 2 colours are given in table 2.

The cycle indices for the action on the set of vertices can be applied to investigate the $C_{60}H_{60}$-molecule. Consider a colouring of the 60 vertices C with 2 colours H or Cl. In other words a colouring is a function f from the set of vertices of the truncated icosahedron into the set $\{\mathrm{H}, \mathrm{Cl}\}$. Then Pólyas theorem says that the number of $C_{60}H_kCl_{60-k}$ molecules is given as the coefficient of x^k in the expansion of the cycle index of the symmetry group $\mathcal{R}$ or $\mathcal{S}$ acting on the set of vertices when all the indeterminates x_i are replaced by $1+x^i$. (In mathematical terms we are speaking of weighted enumeration when we define the weight of a colouring as a *product weight*. Let $w(\mathrm{H}) = x$ and $w(\mathrm{Cl}) = 1$, where x is an indeterminate over the set of rationals. Then the product weight of the colouring f is defined to be

$$w(f) := \prod_v f(v),$$

where the product runs over all vertices v.) In table 3 you can find the numbers of *different* molecules $C_{60}H_kCl_{60-k}$ both for the symmetry groups $\mathcal{R}$ and $\mathcal{S}$.

The substitution $x_i \mapsto 1 + x^i$ into the cycle index is implemented in SYMMETRICA as well. It is called `polya_sub(a,b,c)`, where `a` is the cycle index, `b` is the number of

k	$\mathcal{S}$	$\mathcal{R}$
0, 60	1	1
1, 59	1	1
2, 58	23	37
3, 57	303	577
4, 56	4 190	8 236
5, 55	45 718	91 030
6, 54	418 470	835 476
7, 53	3 220 218	6 436 782
8, 52	21 330 558	42 650 532
9, 51	123 204 921	246 386 091
10, 50	628 330 629	1 256 602 779

Table 3: Number of $C_{60}H_kCl_{60-k}$ molecules

indeterminates x_i that should be replaced by $1 + x^i$ and c is the result of the expansion of the cycle index.
More or less in the same way the numbers of *hetero fullerenes*, these are fullerenes where some of the carbon atoms are replaced by other atoms, can be computed from the cycle index of the symmetry group acting on the set of vertices. For instance replacing some C atoms by B atoms the numbers in table 3 can be interpreted as the numbers of *different* $C_{60-k}B_k$ molecules.
Finally let us investigate the resonance structure of the fullerene C_{60}. For doing this we have to place 30 double bonds and 60 single bonds into the truncated icosahedron, such that each vertex is incident with 2 single bonds and 1 double bond. Obviously it is enough to find the positions of all the double bonds. So we have to determine all sets consisting of exactly 30 edges of the fullerene, such that each vertex is incident with exactly one edge. Applying a SYMMETRICA program which uses a backtrack algorithm it is possible to compute a list of all 12500 possibilities to do that. (It is already known in literature [19] that there are 12500 resonance structures of the fullerene C_{60}.) But many of these structures coincide when applying a symmetry operation on the truncated icosahedron. The symmetry groups $\mathcal{R}$ or $\mathcal{S}$ act as permutation groups on the set of all edges of the fullerene, so they act on the set consisting of all 30-sets of edges as well. Especially they act on the set of all resonance structures. Since the backtrack algorithm above yields a complete set of all structures we can take a constructive approach to compute not only the number of all the *essentially different* resonance structures, but a representative of each of these structures and the symmetry groups of all these representatives as well. This method is a constructive approach for the determination of the number of classes of Kekulé structures of C_{60}. In [7] it is stated that this number could be computed by using the inclusion exclusion formula. Let me give the mathematical background for the constructive approach. Each 30-set A of edges (and according to the remark above each resonance structure) can be identified with its *characteristic function* which is a function χ_A from the set of edges into the set $\{0,1\}$, such that $\chi_A(e) = 1$ if and only if $e \in A$. Using a labelling of the edges with labels $1, \ldots, 90$ these functions can be written as tuples $(\chi_A(1), \ldots, \chi_A(90))$. The set of these 90-tuples is totally ordered by the lexicographic

ordering. The permutation representation of the groups $\mathcal{R}$ or $\mathcal{S}$ on the set of 30-sets of edges can be rewritten as a group action on the set of these characteristic functions induced by a group action on the domain. Choosing as a canonical representative the lexicographic smallest member of its orbit, we can apply standard algorithms to compute a list of all *different* resonance structures from the list of all 12500 resonance structures. Together with each representative we also get its *stabilizer* which is its symmetry group. Since all the elements in one orbit have conjugated stabilizers we can associate an orbit with the conjugacy class $\widetilde{U}$ of the stabilizer U of any orbit representative and we say that the orbit is of *stabilizer type* $\widetilde{U}$. Using the computer algebra system GAP [17] it is possible to derive that there are 22 conjugacy classes $\widetilde{U}$ of subgroups $U \leq \mathcal{S}$. In table 4 all the conjugacy classes $\widetilde{U}$ of $\mathcal{S}$ are listed by giving the point group symbol of a representative together with the size of the class $\widetilde{U}$ (i.e. number of subgroups conjugated to U), the size of U (i.e. the number of elements in the subgroup U) and the number of orbits of resonance structures of C_{60} of stabilizer type $\widetilde{U}$. Summarising, there are 158 (260) different resonance structures with respect to the symmetry group $\mathcal{S}$ (or $\mathcal{R}$ respectively). A list of all the conjugacy classes of subgroups of the icosahedral point group I_h together with the *table of marks* and the *Burnside-matrix* of I_h can be found in [14].

U	$\lvert U\rvert$	$\lvert\widetilde{U}\rvert$	#	U	$\lvert U\rvert$	$\lvert\widetilde{U}\rvert$	#
C_1	1	1	70	C_{3v}	6	10	3
C_i	2	1	0	D_{2h}	8	5	0
C_2	2	15	19	C_{5v}	10	6	1
C_s	2	15	36	D_5	10	6	0
C_3	3	10	7	C_{5i}	10	6	0
D_2	4	5	3	T	12	5	1
C_{2v}	4	15	5	D_{3d}	12	10	3
C_{2h}	4	15	3	D_{5d}	20	6	2
C_5	5	6	0	T_h	24	5	1
D_3	6	10	2	I	60	1	0
C_{3i}	6	10	1	I_h	120	1	1

Table 4: Resonance structures of the C_{60} fullerene

The SYMMETRICA routine `all_orbits_right_from_vector(a,b,c)` computes a complete list `c` of these representatives. The permutation group acting on the domain of the functions is given by `a`, which is a `VECTOR` of generators, which must be `PERMUTATION`-objects. The `VECTOR` `b` is a list of all the functions which must be tested to be a canonical representative or not. The list of all canonical representatives will be computed as the `VECTOR` `c`. For our problem of determining all the *different* resonance structures we have to take for `a` a `VECTOR` of the generators of the symmetry group acting on the set of edges of the truncated icosahedron. And for `b` we have to take the `VECTOR` of all the 12500 resonance structures generated by the backtrack algorithm described above.

Balasubramanian extensively applied Pólya theory for the enumeration of isomers. He published a review on chemical and spectroscopic applications of this theory in [1]. In [2, 3, 7] he computes the cycle indices of the symmetry group of C_{60} acting on its sets of vertices, edges or faces, and he demonstrates how to enumerate isomers of the

form $C_{60}H_n$ and $C_{60}H_nD_m$. Furthermore he computes the numbers of face and edge colourings of C_{60} and determines the nuclear–spin statistics for C_{60} and $C_{60}H_{60}$. When actually computing the numbers of isomers given in his papers he reports that he had to face complexity problems and arithmetic overflows occurred. So he had to implement a double precision arithmetic into his algorithm. When using SYMMETRICA all these problems do not occur, since SYMMETRICA is working with integers of arbitrary length and with rational numbers stored as fractions.
FUJITA [15] computes the numbers of colourings of the truncated icosahedron by *stabilizer type*. He derives the cycle index of $\mathcal{S}$ acting on the set of vertices of C_{60} by summing over so called *partial cycle indices* for certain subgroups of $\mathcal{S}$. (For more details on partial cycle indices see [16].)

4 A multi-dimensional cycle index

Whenever a group G is acting on sets $X_1, \ldots, X_n$ then G acts in a natural way on the disjoint union

$$X := \dot{\bigcup_{i=1}^{n}} X_i.$$

Replacing in such a situation the cycle index of G acting on X by a so-called *n-dimensional* cycle index we get more information about the permutation representation of G. The n-dimensional cycle index which uses for each set X_i a separate family of indeterminates $x_{i,1}, x_{i,2}, \ldots$ is given by

$$Z_n(G, X_1 \dot\cup \ldots \dot\cup X_n) := \frac{1}{|G|} \sum_{g \in G} \prod_{i=1}^{n} \left(\prod_{j=1}^{|X_i|} x_{i,j}^{a_{i,j}(g)} \right),$$

where $(a_{i,1}(g), \ldots, a_{i,|X_i|}(g))$ is the cycle type of the permutation corresponding to g acting on X_i.
Returning to the fullerene C_{60} the groups $\mathcal{R}$ and $\mathcal{S}$ are acting on the disjoint union of the sets of all vertices, pentagonal edges, hexagonal edges, pentagonal faces, hexagonal faces and diagonals. When denoting the families of indeterminates for these actions by the following symbols v_i, e_i, E_i, f_i, F_i and d_i we compute:

$$Z_6(\mathcal{R}) = \frac{1}{60}\Big(24v_5^{12}e_5^{12}E_5^6 f_1^2 f_5^2 F_5^4 d_5^6 + 20v_3^{20}e_3^{20}E_3^{10} f_3^4 F_1^2 F_3^6 d_3^{10} + 15v_2^{30}e_2^{30}E_1^2 E_2^{14} f_2^6 F_2^{10} d_1^2 d_2^{14} + v_1^{60}e_1^{60}E_1^{30} f_1^{12} F_1^{20} d_1^{30}\Big)$$

and

$$Z_6(\mathcal{S}) = \frac{1}{2}Z_6(\mathcal{R}) + \frac{1}{120}\Big(24v_{10}^6 e_{10}^6 E_{10}^3 f_2 f_{10} F_{10}^2 d_5^6 + 20v_6^{10}e_6^{10}E_6^5 f_6^2 F_2 F_6^3 d_3^{10} + 15v_1^4 v_2^{28} e_1^4 e_2^{28} E_1^4 E_2^{13} f_1^4 f_2^4 F_1^4 F_2^8 d_1^2 d_2^{14} + v_2^{30}e_2^{30}E_2^{15} f_2^6 F_2^{10} d_1^{30}\Big).$$

From these cycle indices we deduce that the action on the sets of vertices and pentagonal edges have the same cycle type. The variables E_i, f_i and F_i determine the cycle index of the symmetry group of the icosahedron acting on its set of edges, vertices or faces. Using these 6-dimensional cycle indices we can compute the number of *different* simultaneous colourings of all vertices, pentagonal and hexagonal edges, pentagonal and hexagonal faces and diagonals with $k_1, k_2, \ldots, k_6$ colours by replacing each variable v_i by k_1, e_i by k_2 and so on. For $k_1 = \ldots = k_6 = 2$ the number of $\mathcal{R}$-different colourings is

$$109\,700\,303\,821\,413\,736\,143\,664\,612\,170\,571\,163\,303\,931\,905\,179\,435\,773\,317\,873\,664$$

whereas the number of $\mathcal{S}$-different colourings is

$$54\,850\,151\,910\,706\,868\,071\,832\,306\,128\,208\,569\,015\,853\,860\,985\,570\,356\,157\,743\,104.$$

This substitution into an n-dimensional cycle index can be computed using the SYMMETRICA routine `polya_multi_const_sub(a,b,c)`.

5 Implementation in SYMMETRICA

All the cycle indices for the action of the symmetry group of the fullerene C_{60} are implemented in SYMMETRICA. The 6-dimensional cycle indices for $\mathcal{R}$ and $\mathcal{S}$ are

```
INT zykelind_full60(a) OP a;
INT zykelind_full60_extended(a) OP a;
```

The cycle indices for the actions on the sets of vertices, faces, edges and diagonals are

```
INT zykelind_full60_vertices(a) OP a;
INT zykelind_full60_vertices_extended(a) OP a;
INT zykelind_full60_edges(a) OP a;
INT zykelind_full60_edges_extended(a) OP a;
INT zykelind_full60_faces(a) OP a;
INT zykelind_full60_faces_extended(a) OP a;
INT zykelind_full60_diagonals(a) OP a;
```

In all these cases the `_extended` versions are the cycle indices of the full symmetry group $\mathcal{S}$.

Let me give a short description how to handle polynomials with variables in several alphabets. In SYMMETRICA there is a routine which allows to multiply two polynomials in disjoint sets of indeterminates. The corresponding routine is called

```
INT mult_disjunkt_polynom_polynom(a,b,c) OP a,b,c;
```

where `a` and `b` are the two polynomials that should be multiplied. `c` is the result. A `POLYNOM` object in SYMMETRICA consists of three parts:

- A coefficient,
- the so called *self-part*, which is a `VECTOR` of `INTEGER` objects that represent the exponents of the monomial summands,
- and a *next-part*, which is the lexicographically next monomial, or zero, if there is no further monomial summand of the polynomial in question.

The routine for multiplication of two polynomials in disjoint sets of indeterminates works in the following way: At first the number of variables of the first polynomial `a` is evaluated. (Let this number be n.) Then for each monomial summand of `a` it is tested, if its self-part is of length less than n, and if this is so, then this self-part is changed into a `VECTOR` object of length n and all the new entries are set to zero. Then the self part of each monomial summand of `b` is appended to the self-part of `a` (of length n), forming a new self-part of a monomial summand of `c`. The corresponding coefficients of the monomials of `a` and `b` are multiplied to get the new coefficient of this monomial.
In order to work with these polynomials in two or more alphabets it is therefore important to know how many variables are in the first alphabet, in the second alphabet and so on. Or in other words, we must keep in mind at which index of the self-part of the monomial summands the different alphabets start. (The index where the i-th family starts, is the number of variables which have already occurred in the previous $i-1$ families.) Using a vector of `INTEGER` objects, where for each polynomial the position in the self-parts of the monomial summands is indicated, where the new alphabet starts, gives the whole information. For example consider two polynomials `a` and `b` in two different alphabets (`a` is a polynomial in x_i and `b` is a polynomial in y_i) where `a` has n variables. Then applying `mult_disjunkt_polynom_polynom(a,b,c)` makes `c` to be a polynomial in two families of variables and the corresponding vector of starting points would be $[0, n]$. A monomial summand of `c` can be interpreted as

$$s\_po\_k(c)\prod_{i=0}^{n-1} x_{i+1}^{s\_po\_ii(c,i)} \prod_{i=n}^{s\_po\_li(c)-1} y_{i-n+1}^{s\_po\_ii(c,i)}.$$

For that reason a multi dimensional cycle index in SYMMETRICA consists of a `VECTOR`-part and a `POLYNOM`-part, which can be selected by

```
OP s_mz_v(a) OP a;      OP s_mz_po(a) OP a;
```

The cycle indices for the actions on the sets of vertices, edges, etc. were computed from the 6-dimensional cycle indices by extracting and identifying some families of indeterminates. This extraction of some families of indeterminates of a multi dimensional cycle index can be done by

```
INT mz_extrahieren(a,b,c) OP a,b,c; ,
```

where `a` is a multi dimensional cycle index and `b` is a `VECTOR` object. Its length tells how many families shall be combined into the new cycle index `c`. The entries of `b` are `INTEGER` objects. If for instance `a` is a 6-dimensional cycle index and you want to extract the first and fifth family of indeterminates then `b` would be the `VECTOR` $[1, 5]$ of length 2. In the case you choose only one family to be extracted the result will be a `POLYNOM` object, otherwise it is a multi dimensional cycle index as described above.
For identifying different alphabets there is the routine

```
INT mz_vereinfachen(a,b) OP a,b;
```

which computes from a multi dimensional cycle index `a` a cycle index `b` in only one alphabet. For instance for computing the cycle index of the action on the set of faces of the fullerene, we first extract the two families corresponding to f_i and F_i and then identify f_i and F_i.

```
zykelind_full60(a);  /* 6-dimensional cycle index */
M_IL_V(2L,b);
M_I_I(4L,S_V_I(b,0L));
M_I_I(5L,S_V_I(b,1L));
mz_extrahieren(a,b,c); /* extracting the families 4 and 5 from a */
mz_vereinfachen(c,d);  /* identifying the two alphabets */
```

In addition to this it should be mentioned that the cycle indices of the symmetry groups of the tetrahedron, the cube and the dodecahedron are implemented in the same way in SYMMETRICA.

6 Some further fullerenes

In general molecules in the form of cage-like polyhedra solely built from carbon atoms are called fullerenes. Fullerenes C_n can be constructed for $n = 20$ and for all even $n \geq 24$. They have n vertices (i.e. C-atoms), $3n/2$ edges, 12 pentagonal and $(n-20)/2$ hexagonal faces. The most important member of the family of the fullerenes is C_{60}.
The smallest fullerene is C_{20}, which has no hexagonal faces. The atoms of the C_{20} are positioned at the vertices of a *pentagon dodecahedron*, so the symmetry group of C_{20} is isomorphic to the symmetry group of C_{60}. The generators for $\mathcal{R}(\mathrm{C}_{20})$, the group of all rotational symmetries, acting on the set of vertices are given by

$$\pi_1 = (1,2,3,4,5)(6,7,8,9,10)(11,12,13,14,15)(16,17,18,19,20)$$

and

$$\pi_2 = (1,7,17,19,10)(2,12,18,14,5)(3,8,13,9,4)(6,11,16,20,15).$$

To get the group $\mathcal{S}(\mathrm{C}_{20})$ we have to add a third generator, a reflection

$$\sigma = (1)(2,5)(3,4)(6)(7,10)(8,9)(11,15)(12,14)(13)(16,20)(17,19)(18).$$

The 3-dimensional cycle indices for the action on the sets of vertices, edges and faces are

$$Z_3(\mathcal{R}(\mathrm{C}_{20})) = \frac{1}{60}\left(v_1^{20}e_1^{30}f_1^{12} + 20v_1^2v_3^6e_3^{10}f_3^4 + 15v_2^{10}e_1^2e_2^{14}f_2^6 + 24v_5^4e_5^6f_1^2f_5^2\right)$$

$$Z_3(\mathcal{S}(\mathrm{C}_{20})) = \frac{1}{2}Z_3(\mathcal{R}(\mathrm{C}_{20})) + \frac{1}{120}\left(v_2^{10}e_2^{15}f_2^6 + 20v_2v_6^3e_6^5f_6^2 + 15v_1^4v_2^8e_1^4e_2^{13}f_1^4f_2^4 + 24v_{10}^2e_{10}^3f_2f_{10}\right).$$

In [12, 13] a method is described how to construct a fullerene C_{3n} from a fullerene C_n having the same or even a bigger symmetry group as C_n. This method is called the *Leapfrog principle*. If we are starting with a C_n cluster with icosahedral symmetry all the new clusters will be of the same symmetry, since this is the biggest symmetry group in 3-dimensional space. In the first step you have to put an extra vertex into the centre of each face of C_n. Then connect these new vertices with all the vertices surrounding the corresponding face. Then the dual polyhedron is again a fullerene having $3n$ vertices 12 pentagonal and $(3n/2) - 10$ hexagonal faces. Knowing the 3-dimensional cycle index of $\mathcal{S}(\mathrm{C}_n)$ acting on the sets of vertices, edges and faces it is very easy to compute the cycle index for the induced action of $\mathcal{S}(\mathrm{C}_n)$ on the set of vertices of C_{3n}. We just have to

identify the vertices of C_n with the n new hexagonal faces of C_{3n}. This can be done by identifying the two families of indeterminates describing the action on the sets of vertices and faces of C_n.
For computing the cycle indices for the action on the sets of vertices and edges of C_{3n} we have to proceed in the following way: Let π be an element of $\mathcal{S}(\mathrm{C}_n)$ given as a permutation of the vertices of C_n and π_f the induced permutation of the faces of C_n. Then $\hat{\pi}$, a permutation representation of π acting on the faces of C_{3n}, can be defined as

$$\hat{\pi}(i) := \begin{cases} \pi(i) & \text{if } i \leq n \\ \pi_f(i-n)+n & \text{if } i > n. \end{cases}$$

The permutation representation of π acting on the set of edges of C_{3n} is the induced operation of $\hat{\pi}$ on the union

$$\{\{i,j\} \mid \{i,j\} \text{ is an edge of } \mathrm{C}_n\} \bigcup \{(i,k) \mid i \text{ is a vertex of the face } k-n \text{ in } \mathrm{C}_n\}.$$

In the same way the permutation representation of π acting on the set of vertices of C_{3n} is the induced operation of $\hat{\pi}$ acting on

$$\{(\{i,j\},k) \mid \{i,j\} \text{ is an edge of the face } k-n \text{ in } \mathrm{C}_n\}.$$

From these permutation representations the cycle indices for the action on the sets of vertices or edges can be computed. For instance the C_{60} can be constructed from the C_{20} by the Leapfrog principle.
Besides C_{60} the most prominent fullerene is C_{70}, which has $\mathrm{D}_{5\mathrm{h}}$ as its symmetry group. The C_{70} can be constructed from the C_{60} by cutting the C_{60} along the edges given by the following sequence of vertices: 21, 31, 32, 22, 23, 33, 34, 24, 25, 35, 36, 26, 27, 37, 38, 28, 29, 39, 40, 30, 21. (Again we use the labelling given in figure 2.) Then we have two halves of the truncated icosahedron; the vertices in the first half will be labelled by 1, 2, ..., 40, the vertices of the second half by 21', 22', ..., 60'. Now lift the upper half, turn it by an angle of $\pi/5$ such that we get 5 new hexagons with labels

$$\begin{array}{llllll} 21'=32, & 22, & 23, & 22'=33, & 32', & 31' \\ 23'=34, & 24, & 25, & 24'=35, & 34', & 33' \\ 25'=36, & 26, & 27, & 26'=37, & 36', & 35' \\ 27'=38, & 28, & 29, & 28'=39, & 38', & 37' \\ 29'=40, & 30, & 21, & 30'=31, & 40', & 39' \end{array}$$

Since ten of the labels of the vertices in the first half coincide with ten of the labels in the second half there are only 70 vertices (but 80 labels). The group of rotational symmetries is given by one 5-fold rotation π_1 and five 2-fold rotations. Combining these rotations with one reflection σ gives the group of all symmetries. Renaming the labels i' by $i+10$ for $i \geq 31$, the generators for these two groups acting on the set of vertices are given by:
$\pi_1 =$ (66,67,68,69,70)(61,62,63,64,65)(52,54,56,58,60)(51,53,55,57,59)(42,44,46,48,50)
(41,43,45,47,49)(32,34,36,38,40)(31,33,35,37,39)(22,24,26,28,30)(21,23,25,27,29)
(12,14,16,18,20)(11,13,15,17,19)(6,7,8,9,10)(1,2,3,4,5)
$\pi_2 =$ (37,38)(36,39)(35,40)(32,33)(31,34)(30,44)(29,45)(28,46)(27,47)(26,48)(25 ,49)
(24,50)(23,41)(22,42)(21,43)(20,54)(19,55)(18,56)(17,57)(16,58)(15,59)(14,60)(13,51)
(12,52)(11,53)(10,63)(9,64)(8,65)(7,61)(6,62)(5,68)(4,69)(3,70)(2,66)(1,67)

$\sigma =$ (70)(67,68)(66,69)(65)(62,63)(61,64)(59,60)(54,55)(53,56)(52,57)(51,58)(49,50) (44,45)(43,46)(42,47)(41,48)(35,36)(34,37)(33,38)(32,39)(31,40)(25,26)(24,27)(23,28) (22,29)(21,30)(15,16)(14,17)(13,18)(12,19)(11,20)(8,9)(7,10)(6)(3,4)(2,5)(1)

Finally the 3-dimensional cycle indices for the action on the sets of vertices, edges and faces are

$$Z_3(\mathcal{R}(\mathrm{C}_{70})) = \frac{1}{10}\left(4v_5^{14}e_5^{21}f_1^2f_5^7 + 5v_2^{35}e_1e_2^{52}f_1f_2^{18} + v_1^{70}e_1^{105}f_1^{37}\right)$$

$$Z_3(\mathcal{S}(\mathrm{C}_{70})) = \frac{1}{2}Z_3(\mathcal{R}(\mathrm{C}_{70})) + \frac{1}{20}\left(4v_5^2v_{10}^6e_5e_{10}^{10}f_2f_5f_{10}^3 + 5v_1^4v_2^{33}e_1^9e_2^{48}f_1^9f_2^{14} + v_1^{10}v_2^{30}e_1^5e_2^{50}f_1^5f_2^{16}\right).$$

In [6] and [5] huge tables with numbers of isomers and of chiral isomers of substituted fullerenes from C_{20} to C_{70} are computed, but the corresponding cycle indices are not given. In [9] an even greater list of fullerene structures can be found. The cycle indices of the symmetry groups of these fullerenes can be computed by determining the permutation representation of the symmetry groups of these fullerenes acting on their sets of vertices, edges or faces. Here we want to present a list of the 3-dimensional cycle indices for these fullerenes.

The point group of C_{24} is $\mathrm{D}_{6\mathrm{d}}$ which leads to the following cycle indices.

$$Z_3(\mathcal{R}(\mathrm{C}_{24})) = \frac{1}{12}\left(2e_6^6f_1^2f_6^2v_6^4 + 2e_3^{12}f_1^2f_3^4v_3^8 + e_2^{18}f_1^2f_2^6v_2^{12} + 6e_1^2e_2^{17}f_2^7v_2^{12} + e_1^{36}f_1^{14}v_1^{24}\right)$$

$$Z_3(\mathcal{S}(\mathrm{C}_{24})) = \frac{1}{2}Z_3(\mathcal{R}(\mathrm{C}_{24})) + \frac{1}{24}\left(4e_{12}^3f_2f_{12}v_{12}^2 + 2e_4^9f_2f_4^3v_4^6 + 6e_1^4e_2^{16}f_1^4f_2^5v_1^4v_2^{10}\right).$$

Since the C_{26} has a symmetry group of the form $\mathrm{D}_{3\mathrm{h}}$ we have

$$Z_3(\mathcal{R}(\mathrm{C}_{26})) = \frac{1}{6}\left(3e_1e_2^{19}f_1f_2^7v_2^{13} + 2e_3^{13}f_3^5v_1^2v_3^8 + e_1^{39}f_1^{15}v_1^{26}\right)$$

$$Z_3(\mathcal{S}(\mathrm{C}_{26})) = \frac{1}{2}Z_3(\mathcal{R}(\mathrm{C}_{26})) + \frac{1}{12}\left(2e_3e_6^6f_3f_6^2v_2v_3^2v_6^3 + 3e_1^5e_2^{17}f_1^5f_2^5v_1^4v_2^{11} + e_1^3e_2^{18}f_1^3f_2^6v_1^6v_2^{10}\right).$$

The fullerene C_{28} is of tetrahedral symmetry T_d so the cycle indices can be computed as

$$Z_3(\mathcal{R}(\mathrm{C}_{28})) = \frac{1}{12}\left(8e_3^{14}f_1f_3^5v_1v_3^9 + 3e_1^2e_2^{20}f_2^8v_2^{14} + e_1^{42}f_1^{16}v_1^{28}\right)$$

$$Z_3(\mathcal{S}(\mathrm{C}_{28})) = \frac{1}{2}Z_3(\mathcal{R}(\mathrm{C}_{28})) + \frac{1}{24}\left(6e_2e_4^{10}f_4^4v_4^7 + 6e_1^4e_2^{19}f_1^4f_2^6v_1^6v_2^{11}\right).$$

The cycle index of $\mathcal{R}(\mathrm{C}_{28})$ acting on its set of vertices can be found in [4] as well.

The C_{30} has $\mathrm{D}_{5\mathrm{h}}$ symmetry and the cycle indices for the action on the sets of edges, faces and vertices are

$$Z_3(\mathcal{R}(\mathrm{C}_{30})) = \frac{1}{10}\left(4e_5^9f_1^2f_5^3v_5^6 + 5e_1e_2^{22}f_1f_2^8v_2^{15} + e_1^{45}f_1^{17}v_1^{30}\right)$$

$$Z_3(\mathcal{S}(\mathrm{C}_{30})) = \frac{1}{2}Z_3(\mathcal{R}(\mathrm{C}_{30})) + \frac{1}{20}\left(4e_5e_{10}^4f_2f_5f_{10}v_{10}^3 + 5e_1^5e_2^{20}f_1^5f_2^6v_1^6v_2^{12} + e_1^5e_2^{20}f_1^5f_2^6v_2^{15}\right).$$

The symmetry group of C_{32} is D_3, so it consists only of rotations and we have

$$Z_3(\mathcal{R}(\mathrm{C}_{32})) = \frac{1}{6}\left(2e_3^{16}f_3^6v_1^2v_3^{10} + 3e_1^2e_2^{23}f_2^9v_2^{16} + e_1^{48}f_1^{18}v_1^{32}\right).$$

Since C_{34} has C_{3v} symmetry the cycle indices are

$$Z_3(\mathcal{R}(C_{34})) = \frac{1}{3}\Big(2e_3^{17}f_1f_3^6v_1v_3^{11} + e_1^{51}f_1^{19}v_1^{34}\Big)$$

$$Z_3(\mathcal{S}(C_{34})) = \frac{1}{2}\Big(Z_3(\mathcal{R}(C_{34})) + e_1^5e_2^{23}f_1^5f_2^7v_1^4v_2^{15}\Big).$$

The point group of C_{36} is D_{6h}, from which the following cycle indices can be computed.

$$Z_3(\mathcal{R}(C_{36})) = \frac{1}{12}\Big(2e_6^9f_2f_6^3v_6^6 + 2e_3^{18}f_1^2f_3^6v_3^{12} + 4e_2^{27}f_1^2f_2^9v_2^{18} + 3e_1^2e_2^{26}f_2^{10}v_2^{18} + e_1^{54}f_1^{20}v_1^{36}\Big)$$

$$Z_3(\mathcal{S}(C_{36})) = \frac{1}{2}Z_3(\mathcal{R}(C_{36})) + \frac{1}{24}\Big(2e_3^2e_6^8f_2f_3^2f_6^2v_6^6 + e_2^{27}f_2^{10}v_2^{18} + 2e_6^9f_1^2f_6^3v_6^6 +$$
$$3e_1^4e_2^{25}f_1^4f_2^8v_1^8v_2^{14} + 3e_1^6e_2^{24}f_1^6f_2^7v_1^4v_2^{16} + e_1^6e_2^{24}f_1^6f_2^7v_2^{18}\Big).$$

C_{38} is of C_{3v} symmetry so we have

$$Z_3(\mathcal{R}(C_{38})) = \frac{1}{3}\Big(2e_3^{19}f_3^7v_1^2v_3^{12} + e_1^{57}f_1^{21}v_1^{38}\Big)$$

$$Z_3(\mathcal{S}(C_{38})) = \frac{1}{6}\Big(2e_3^{19}f_3^7v_1^2v_3^{12} + 3e_1^5e_2^{26}f_1^5f_2^8v_1^6v_2^{16} + e_1^{57}f_1^{21}v_1^{38}\Big).$$

For the C_{40} two possible symmetry groups are given, namely T_d and D_{5d}. In the first case the cycle indices are

$$Z_3(\mathcal{R}(C_{40})) = \frac{1}{12}\Big(3e_2^{30}f_1^2f_2^{10}v_2^{20} + 8e_3^{20}f_1f_3^7v_1v_3^{13} + e_1^{60}f_1^{22}v_1^{40}\Big)$$

$$Z_3(\mathcal{S}(C_{40})) = \frac{1}{2}Z_3(\mathcal{R}(C_{40})) + \frac{1}{24}\Big(6e_4^{15}f_2f_4^5v_4^{10} + 6e_1^6e_2^{27}f_1^6f_2^8v_1^4v_2^{18}\Big).$$

For the symmetry group D_{5d} we compute

$$Z_3(\mathcal{R}(C_{40})) = \frac{1}{10}\Big(4e_5^{12}f_1^2f_5^4v_5^8 + 5e_1^2e_2^{29}f_2^{11}v_2^{20} + e_1^{60}f_1^{22}v_1^{40}\Big)$$

$$Z_3(\mathcal{S}(C_{40})) = \frac{1}{2}Z_3(\mathcal{R}(C_{40})) + \frac{1}{20}\Big(4e_{10}^6f_2f_{10}^2v_{10}^4 + e_2^{30}f_2^{11}v_2^{20} + 5e_1^6e_2^{27}f_1^6f_2^8v_1^4v_2^{18}\Big).$$

Since the point group of C_{42} is D_3 we have

$$Z_3(\mathcal{R}(C_{42})) = \frac{1}{6}\Big(2e_3^{21}f_1^2f_3^7v_3^{14} + 3e_1e_2^{31}f_1f_2^{11}v_2^{21} + e_1^{63}f_1^{23}v_1^{42}\Big).$$

For the D_{3h} symmetry group of C_{44} we can compute

$$Z_3(\mathcal{R}(C_{44})) = \frac{1}{6}\Big(2e_3^{22}f_3^8v_1^2v_3^{14} + 3e_1^2e_2^{32}f_2^{12}v_2^{22} + e_1^{66}f_1^{24}v_1^{44}\Big)$$

$$Z_3(\mathcal{S}(C_{44})) = \frac{1}{2}Z_3(\mathcal{R}(C_{44})) + \frac{1}{12}\Big(2e_3^2e_6^{10}f_3^2f_6^3v_2v_3^2v_6^6 + 4e_1^6e_2^{30}f_1^6f_2^9v_1^6v_2^{19}\Big).$$

A second form of C_{44} is chiral and has T as its symmetry group which gives the following cycle index:

$$Z_3(\mathcal{R}(C_{44})) = \frac{1}{12}\Big(3e_1^2e_2^{32}f_2^{12}v_2^{22} + 8e_3^{22}f_3^8v_1^2v_3^{14} + e_1^{66}f_1^{24}v_1^{44}\Big).$$

The symmetry group of C_{46} is C_3 so we compute

$$Z_3(\mathcal{R}(C_{46})) = \frac{1}{3}\Big(2e_3^{23}f_1f_3^8v_1v_3^{15} + e_1^{69}f_1^{25}v_1^{46}\Big).$$

The C_{48} has D_3 as its symmetry group, so we have

$$Z_3(\mathcal{R}(C_{48})) = \frac{1}{6}\Big(2e_3^{24}f_1^2f_3^8v_3^{16} + 3e_1^2e_2^{35}f_2^{13}v_2^{24} + e_1^{72}f_1^{26}v_1^{48}\Big).$$

For the D_{5h} symmetry of C_{50} we derive

$$Z_3(\mathcal{R}(C_{50})) = \frac{1}{10}\Big(4e_5^{15}f_1^2f_5^5v_5^{10} + 5e_1e_2^{37}f_1f_2^{13}v_2^{25} + e_1^{75}f_1^{27}v_1^{50}\Big)$$

$$Z_3(\mathcal{S}(C_{50})) = \frac{1}{2}Z_3(\mathcal{R}(C_{50})) + \frac{1}{20}\Big(4e_5e_{10}^7f_2f_5f_{10}^2v_5^2v_{10}^4 + 5e_1^7e_2^{34}f_1^7f_2^{10}v_1^4v_2^{23} + e_1^5e_2^{35}f_1^5f_2^{11}v_1^{10}v_2^{20}\Big).$$

The symmetry group of C_{52} is T, which consists only of rotational symmetries.

$$Z_3(\mathcal{R}(C_{52})) = \frac{1}{12}\Big(3e_1^2e_2^{38}f_2^{14}v_2^{26} + 8e_3^{26}f_1f_3^9v_1v_3^{17} + e_1^{78}f_1^{28}v_1^{52}\Big).$$

C_{54} has point group D_3, so we compute

$$Z_3(\mathcal{R}(C_{54})) = \frac{1}{6}\Big(3e_1e_2^{40}f_1f_2^{14}v_2^{27} + 2e_3^{27}f_1^2f_3^9v_3^{18} + e_1^{81}f_1^{29}v_1^{54}\Big).$$

For the D_{3d} symmetry group of C_{56} the cycle indices are

$$Z_3(\mathcal{R}(C_{56})) = \frac{1}{6}\Big(2e_3^{28}f_3^{10}v_1^2v_3^{18} + 3e_1^2e_2^{41}f_2^{15}v_2^{28} + e_1^{84}f_1^{30}v_1^{56}\Big)$$

$$Z_3(\mathcal{S}(C_{56})) = \frac{1}{2}Z_3(\mathcal{R}(C_{56})) + \frac{1}{12}\Big(2e_6^{14}f_6^5v_2v_6^9 + 3e_1^6e_2^{39}f_1^6f_2^{12}v_1^8v_2^{24} + e_2^{42}f_2^{15}v_2^{28}\Big).$$

The symmetry group of C_{58} is C_{3v} so we have

$$Z_3(\mathcal{R}(C_{58})) = \frac{1}{3}\Big(2e_3^{29}f_1f_3^{10}v_1v_3^{19} + e_1^{87}f_1^{31}v_1^{58}\Big)$$

$$Z_3(\mathcal{S}(C_{58})) = \frac{1}{2}\Big(Z_3(\mathcal{R}(C_{58})) + e_1^7e_2^{40}f_1^7f_2^{12}v_1^6v_2^{26}\Big).$$

C_{80} is the next fullerene with I_h symmetry. Its cycle index is

$$Z_3(\mathcal{R}(C_{80})) = \frac{1}{60}\Big(24e_5^{24}f_1^2f_5^8v_5^{16} + 20e_3^{40}f_3^{14}v_1^2v_3^{26} + 15e_2^{60}f_1^2f_2^{20}v_2^{40} + e_1^{120}f_1^{42}v_1^{80}\Big)$$

$$Z_3(\mathcal{S}(C_{80})) = \frac{1}{2}Z_3(\mathcal{R}(C_{80})) + \frac{1}{120}\Big(e_2^{60}f_2^{21}v_2^{40} + 20e_6^{20}f_6^7v_2v_6^{13} + 15e_1^8e_2^{56}f_1^8f_2^{17}v_1^8v_2^{36} + 24e_{10}^{12}f_2f_{10}^4v_{10}^8\Big).$$

The first fullerene with symmetry group I is the C_{140}. Its cycle index is

$$Z_3(\mathcal{R}(C_{140})) = \frac{1}{60}\Big(24e_5^{42}f_1^2f_5^{14}v_5^{28} + 20e_3^{70}f_3^{24}v_1^2v_3^{46} + 15e_1^2e_2^{104}f_2^{36}v_2^{70} + e_1^{210}f_1^{72}v_1^{140}\Big)$$

We could go on listing the cycle indices of many more fullerenes. In many cases it is possible to arrange the n vertices of C_n in several different ways leading to different symmetry groups and to different cycle indices. For instance for the fullerene C_{78} there are 4 possible isomers given in [9]. So from chemical properties we first have to determine the actual shape of the molecule. In [11] it is shown that C_{76} is of D_2 symmetry and not of T_d symmetry which would be possible as well.
You can try to determine generators and cycle indices for various fullerenes C_n and the numbers of *different* colourings of them by using some SYMMETRICA programs[1] at the authors homepage[2].

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