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ORIGINAL PAPER

Enumeration of substitutional isomers with restrictive mutual positions of ligands. II. Counts with restrictions on (sub)symmetry

Vladimir R. Rosenfeld · Douglas J. Klein

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Abstract The present paper extends our previous discussion of paper I on "Overall Counts", still focusing on enumerations of substitutional isomers with restrictive positioning of ligands. But now, we address the counts of such isomers with a specified subsymmetry of the symmetry of the parent skeleton. Constrained analogs of Pólya's cycle index still appear, but now we introduce more powerful technical tools to include subsymmetry-specified generalizations of the cycle index. This involves differential-operator approach for analytically treating newly derived hybrids of the the generalized cycle index and suitable F-polynomials. As a simple illustration of the general mathematical exposition, a specific problems are solved and some tasks for possible further consideration are also stated, where again the Maple symbolic manipulation package proves useful.

Keywords Enumeration · Substitutional isomers · Restrictive substitution · Symmetry-restrictive · F-polynomials

1 Introduction

Herein, we refer to our general introduction to the subject which was given in the previous part I [1] and now focus on our present work.

V. R. Rosenfeld (✉) · D. J. Klein
Mathematical Chemistry Group, Department of Marine Sciences, Texas A&M University at Galveston, Galveston, TX, 77553–1675, USA
e-mail: rosenfev@tamug.edu; vladimir_rosenfeld@yahoo.com

D. J. Klein
e-mail: kleind@tamug.edu

2 Preliminaries

This section is devoted to an exposition of mathematical notions and tools adopting ideas and notations of the Part I ("Overall Counts").

2.1 Symmetry-specific polynomials of graphs

This part of our text is important for our hybridization and utilization of analogies and relations between Pólya's cycle indices [2–4] and the (family) polynomials of graphs [5–8]. For an arbitrary graph G and a family F of (its) subgraphs, we develop certain hybrid polynomials which possess the features of both types of generating functions, to enumerate vertex covers C (of a graph G with subgraphs $\mathsf{f} \in F$) for different subsymmetries of embedding of subgraphs $\mathsf{f} \in \mathsf{C}$ in G. This program of attention to subsymmetries follows [9–11], and utilizes some additional terminology.

Let a finite permutation group A ($|A| = p$) act on a finite set X ($|X| = n$). By definition, an orbit $X_i(A)$ ($1 \leq i \leq t$), induced by a permutation group A on X is an equivalence class of objects $x \in X$, such that: $x, y \in X_i(A) \Longleftrightarrow$ there exists $g \in A$ such that $gx = y$ (where gx denotes the result of action of permutation g on x). Denote [3] the set

$$A\backslash\backslash X := \{X_1(A), X_2(A), \ldots, X_t(A)\} \tag{1}$$

of all orbits $X_i(A)$ induced by A acting on X. [As an aside, note that in the more general case of semigroups, the definition of an orbit induced by a semigroup cannot always fully obey our condition, a more general definition is possible [10]. Namely, in the case of a semigroup S, an *orbit* $X_i = X_i(S)$ ($1 \leq i \leq t$) is a minimal S-closed subset, of X, such that $\forall h \in S$, $\forall x \in X_i$ and $\forall y \in X \setminus X_i$ we have $hx \in X_i$ and $hy \in X \setminus X_i$. Note that the condition of minimality cannot be relaxed, for otherwise, it would not generally distinguish single orbits from unions thereof.]

A subgroup $H \subseteq A$ was called *closed* and *periodic* by Rota and Smith [12], or *automorphic* synonymously in [11], iff H is the maximum among all subgroups inducing one and the same set of orbits ($\hat{H}\backslash\backslash X$). The closed nature of such a subgroup H will be indicated by a "hat" ($\hat{}$) over the subgroup name, thusly $\hat{H}$. Such an $\hat{H}$ contains all the coorbital subgroups, and $\hat{H}$ is also termed the *closure* of all its coorbital subgroups H.

For each subgroup $H \subseteq A$ and an element $g \in A$, the transformation $H^g = gHg^{-1} = H'$ gives a subgroup in A *conjugate* to H. The notion of subgroup conjugacy permits an economy in practical combinatorial applications of (symmetry) groups, since every pair of conjugated subgroups always produces essentially the same combinatorial action. In particular, for an isomer conformation with symmetry group H and $x \in X_i(H)$, there is another conformation (gx) for the same isomer now having symmetry group H^g, and one may consider the combinatorial actions only of one representative $\hat{H}$ of each conjugacy class $Con(H)$ of subgroups. Then, there always exists a one-to-one correspondence between orbit sets

$H\backslash\backslash X = \{X_1(H), X_2(H), \ldots, X_s(H)\}$ and $H^g\backslash\backslash X = \{X_1(H^g), X_2(H^g), \ldots, X_s(H^g)\}$ such that $|X_i(H)| = |X_i(H^g)|$ $(1 \le i \le s; s \ge t)$.

Now, as a case in point, let $F(G; \mathbf{x}, \mathbf{w})$ be the F-polynomial of a graph $G(X; E)$ with the automorphism group Aut G= Aut$\mathcal{M} \cong A$ and let subgroups $\hat{H}_1, \hat{H}_2, \ldots, \hat{H}_r$ be representatives of all conjugacy classes of closed subgroups in A. Then, we can make the following 'symmetry splitting' of the polynomial $F(G; \mathbf{x}, \mathbf{w})$:

$$F(G; \mathbf{x}, \mathbf{w}) = \sum_{j=1}^{r} F(G; \hat{H}_j; \mathbf{x}, \mathbf{w}), \tag{2}$$

where $F(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$ is the restriction of the F-polynomial for just F-covers C with the automorphism group Aut C for which $(A \cap \text{Aut}\mathsf{C}) \in Con(\hat{H}_j)$. In other words, (2) displays the F-covers C of a graph G in accordance with their induced subsymmetries in G.

We call the polynomial $F(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$ the *symmetry-specific*, or $\hat{H}_j$*-specific polynomial* of G. *E. g.*, the symmetry-specific matching polynomial $M(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$ can be a remarkable analytical tool for keeping and processing combinatorial information concerning substitutional isomers involving both unidentate and bidentate ligands.

To deal with symmetry-specific polynomials $F(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$, one first computes auxiliary polynomials $P(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$ that enumerate all F-covers C for which $\hat{H}_j \subseteq A \cap \text{Aut}\mathsf{C}$. This contrasts with $F(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$ for which $\hat{H}_j = A \cap \text{Aut}\mathsf{C}$. In other words, for $F(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$ substitutional patterns (*i. e.*, F-covers C) have automorphism groups (isomorphic to) $\hat{H}_j$, whereas for $P(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$ the counted substitutional patterns have symmetries with $\hat{H}_j$ being a subgroup. These *symmetry-restricted polynomials* $P(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$ can be calculated using either our original method [11] detailed later here or Burnside's table of marks [3,13]. The most part of all isomer enumerations using the table of marks has been performed by Fujita [14], who published several dozens of papers on this subject. Although the approach employed here [11] is newer than Burnside's and differs in form, all three have the same underlying combinatorial background. Thence, one may choose what is deemed more convenient.

Now, the intermediate polynomials $P(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$ are to be used to calculate the target polynomials $F(G; \hat{H}_j; \mathbf{x}, \mathbf{w})$. First, notice that the set $\mathsf{H} = \{\hat{H}_1, \hat{H}_2, \ldots, \hat{H}_r\}$ of representatives of conjugacy classes of closed subgroups, in A, forms a *poset* (*partially ordered set*) with a "zero" element $\hat{H}_1 = \{e\}$ (where e is the identity) and a "unit" $\hat{H}_r = A$. The relevant partial order $\preceq$ is as follows: For two (not necessarily distinct) subgroups $\hat{H}_i, \hat{H}_j \in \mathsf{H}$ $(1 \le i \le j \le r)$, $\hat{H}_i \preceq \hat{H}_j$ iff (if and only if) there is an $\hat{H}_j' \in Con(\hat{H}_j)$, such that $\hat{H}_i \subseteq \hat{H}_j'$. If $\hat{H}_i \preceq \hat{H}_j$ & $\hat{H}_j \preceq \hat{H}_i$, then $\hat{H}_i$ & $\hat{H}_j$ are isomorphic $(\hat{H}_i \cong \hat{H}_j)$. If $\hat{H}_i \preceq \hat{H}_j$ & $\hat{H}_i \ncong \hat{H}_j$, then $\hat{H}_i \prec \hat{H}_j$.

To obtain the symmetry-specific polynomials from symmetry-reduced ones, the (*combinatorial Riemann*) ζ*-function* and the *Möbius* μ*-function of* H. By definition, the ζ*-function of* H is the function $\zeta : \mathsf{H} \times \mathsf{H} \to \{0, 1\}$ represented by the matrix $\underline{\underline{\zeta}} = \left[\zeta_{ij}\right]_{i,j=1}^{n}$ with entries

$$\zeta_{ij} \equiv \zeta(\hat{H}_i, \hat{H}_j) = \begin{cases} 1, & \text{if } \hat{H}_i \preceq \hat{H}_j \ (1 \le i \le j \le n); \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

The ζ-function nicely describes the hierarchy and subordination of all closed subgroups $\hat{H}_i \in \mathsf{H}$. The μ-function is represented in terms of the matrix inverse to $\underline{\underline{\zeta}}$ [2,3,11]. There exist [15] purely combinatorial algorithms for obtaining μ from ζ.

For instance, consider the ζ-function of the poset H of closed subgroups of the symmetry group T_d of a regular tetrahedron (see Wikipedia and Wolfram in the Internet for more information). A regular tetrahedron has 12 rotational (or orientation-preserving) symmetries, and a total of 24 symmetries including transformations that combine a reflection and a rotation. The group of all symmetries is isomorphic to the symmetric group S_4 (of permutations of 4 objects), since there is exactly one such symmetry operation for each permutation of the vertices of the tetrahedron. The set of orientation-preserving symmetries forms a group referred to as the alternating subgroup A_4 of even permutations of S_4. That the graph of the tetrahedron is isomorphic to the complete graph K_4 allows a determination of the number of closed subgroups of our T_d even before indentification of these subgroups. Namely, there exist 5 partitions of the number four: $4 = 1+1+1+1; 4 = 1+1+2; 4 = 2+2; 4 = 3+1; 4 = 4$. Here, we readily see that the first and last closed subgroups are $\hat{H}_1 = C_1$ and $\hat{H}_5 = T_d$, the conjugacy classes of each containing only one subgroup ($|Con(C_1)| = |Con(T_d)| = 1$). The remaining 3 subgroups are addressed using a (T_d-)decorated cube. For this, we take a cube and draw 6 diagonal lines, one to each of its 6 faces, such that any 2 lines drawn on opposite faces are criss-crossed and each vertex of a cube is incident to either 0 or 3 diagonal lines, where each possibility (0 or 3) occurs 4 times. We thus obtain a tetrahedral-symmetry object. A second subgroup of T_d is C_2 ($|C_2| = 2$; $|Con(C_2)| = 3$), comprised from the unity and a 2-fold rotation around the axis which passes through the centers of opposite faces of our decorated cube. This rotation induces two 2-element orbits on the set of vertices of the tetrahedron and corresponds to simultaneously changing the orientation of two nonincident edges of the tetrahedron and thereby gives the third partition $4 = 2 + 2$. The subgroup C_2 is not, however, closed, and we meet the corresponding closed one among the subsequent subgroups. The next subgroup $C_s^{'}$ ($|C_s^{'}| = 2$; $|Con(C_s^{'})| = 3$) corresponds to a mirror plane crossing in a diagonal direction 2 opposite faces of a cube. This induces two 1-element & one 2-element orbits on the set of vertices of a tetrahedron and corresponds to changing the orientation of exactly one edge of a tetrahedron; that is, we have the second mentioned partition $4 = 1 + 1 + 2$. Here, C_s is itself a closed subgroup $\hat{H}_2$ (which is checkable as an easy exercise). After this, there follows C_3 ($|C_3| = 3$; $|Con(C_3)| = 8$) which is due to a rotation axis of the third order passing along the longest diagonal of a cube, or through one vertex and the center of the opposite face of a tetrahedron. This group yields the fourth partition $4 = 1 + 3$, but is not a closed subgroup. Then, as a group-theoretical union of C_2 and C_s, there arises $C_{2v}^{'}$ ($|C_{2v}^{'}| = 4$; $|Con(C_{2v}^{'})| = 3$); this is the desired closed subgroup $\hat{H}_3$ which corresponds to the third partition $4 = 2 + 2$ and induces the same orbits as C_2 above. The next subgroup C_{3v} ($|C_{3v}| = 6$; $|Con(C_{3v})| = 4$) is the closed subgroup $\hat{H}_4$, which corresponds to the fourth partition of 4 ($4 = 1 + 3$) and induces the same orbits as its subgroup C_3. The higher-ranked subgroups

D_{2d} ($|D_{2d}| = 8, |Con(D_{2d})| = 3$) and T ($|T| = 12; |Con(T)| = 1$) induce only one 4-element orbit corresponding to the fifth (trivial, identical) partition $4 = 4$, for which the group T_d is itself the closed subgroup $\hat{H}_5$.

As a result of our detailed illustrative calculation, we have collected the needed information for the construction of the poset H. We find 5 closed subgroups of T_d, viz.: $\hat{H}_1 = C_1$, $\hat{H}_2 = C_s^{'}$, $\hat{H}_3 = C_{2v}^{'}$, $\hat{H}_4 = C_{3v}$, $\hat{H}_5 = T_d$. For these subgroups, note that $\hat{H}_1 \preceq \hat{H}_1, \hat{H}_2, \hat{H}_3, \hat{H}_4, \hat{H}_5$; $\hat{H}_2 \preceq \hat{H}_2, \hat{H}_3, \hat{H}_4, \hat{H}_5$; $\hat{H}_3 \preceq \hat{H}_3, \hat{H}_5$; $\hat{H}_4 \preceq \hat{H}_4, \hat{H}_5$; $\hat{H}_5 \preceq \hat{H}_5$.

The last conclusions about the order subordination of elements in this poset H contain the necessary and sufficient information for calculating the ζ-function of the poset H. Viz.:

$$\underline{\underline{\zeta}} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ & 1 & 1 & 1 & 1 \\ & & 1 & 0 & 1 \\ & & & 1 & 1 \\ & & & & 1 \end{bmatrix}. \tag{4}$$

The Möbius function of H is obtained through inversion of the matrix $\underline{\underline{\zeta}}$:

$$\underline{\underline{\mu}} = \underline{\underline{\zeta}}^{-1} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ & 1 & -1 & -1 & 1 \\ & & 1 & 0 & -1 \\ & & & 1 & -1 \\ & & & & 1 \end{bmatrix}. \tag{5}$$

Now, the question about the interrelations between graph polynomials $F(G; \hat{H}_i; \mathbf{x}, \mathbf{w})$ and $P(G; \hat{H}_i; \mathbf{x}, \mathbf{w})$ is easy to answer. Let $\mathbf{F}$ (res. $\mathbf{P}$) be a column vector with components $F_i = F(G; \hat{H}_i; \mathbf{x}, \mathbf{w})$ (res. $P_i = P(G; \hat{H}_i; \mathbf{x}, \mathbf{w})$) ($1 \le i \le r$). Then, the solution of our system of simultaneous linear equations ($\mathbf{P} = \underline{\underline{\zeta}}\mathbf{F}$) is

$$\mathbf{F} = \underline{\underline{\zeta}}^{-1}\mathbf{P} = \underline{\underline{\mu}}\mathbf{P}. \tag{6}$$

Making use of an earlier considered example (see (6) in Part I) as a case of the F-polynomial, we can manually compute respective polynomials $P(G; \hat{H}_1; \mathbf{x}, \mathbf{w})$:

$$\begin{aligned} P(K_4; \hat{H}_1; \mathbf{x}, \mathbf{w}) &= x_1x_2x_3x_4 + x_1x_2w_2 + x_1x_3w_2 + x_1x_4w_2 + x_2x_3w_2 + x_2x_4w_2 \\ &\quad + x_3x_4w_2 + 3w_2^2; \\ P(K_4; \hat{H}_2; \mathbf{x}, \mathbf{w}) &= x_1x_2x_3x_4 + x_1x_2w_2 + x_1x_3w_2 + x_1x_4w_2 + x_2x_3w_2 + x_2x_4w_2 \\ &\quad + x_3x_4w_2 + 3w_2^2; \\ P(K_4; \hat{H}_3; \mathbf{x}, \mathbf{w}) &= x_1x_2x_3x_4 + x_1x_2w_2 + x_1x_3w_2 + x_1x_4w_2 + x_2x_3w_2 + x_2x_4w_2 \\ &\quad + x_3x_4w_2 + 3w_2^2; \\ P(K_4; \hat{H}_4; \mathbf{x}, \mathbf{w}) &= x_1x_2x_3x_4; \end{aligned}$$

$$P(K_4; \hat{H}_5; \mathbf{x}, \mathbf{w}) = x_1x_2x_3x_4. \tag{7}$$

From (7), it is seen that the minimum possible subsymmetry of matchings of a regular tetrahedron corresponds to the symmetry subgroup $C_{2v}^{'}$. That is, a priori, the first two components of the column vector $\mathbf{F}$, on the L.H.S. of (6), are 0 ($F_1 = F_2 = 0$). But we want to obtain a complete solution of the system (6), so that we substitute the R.H.S.'s of expressions (7) for respective components $P_j (1 \leq j \leq n)$ of the vector $\mathbf{P}$ in (6) to give

$$\begin{aligned}
\mathbf{F} &= \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ & 1 & -1 & -1 & 1 \\ & & 1 & 0 & -1 \\ & & & 1 & -1 \\ & & & & 1 \end{bmatrix} \cdot \begin{bmatrix} P(K_4; \hat{H}_1; \mathbf{x}, \mathbf{w}) \\ P(K_4; \hat{H}_2; \mathbf{x}, \mathbf{w}) \\ P(K_4; \hat{H}_3; \mathbf{x}, \mathbf{w}) \\ P(K_4; \hat{H}_4; \mathbf{x}, \mathbf{w}) \\ P(K_4; \hat{H}_5; \mathbf{x}, \mathbf{w}) \end{bmatrix} \\
&= \begin{bmatrix} P(K_4; \hat{H}_1; \mathbf{x}, \mathbf{w}) - P(K_4; \hat{H}_2; \mathbf{x}, \mathbf{w}) \\ P(K_4; \hat{H}_2; \mathbf{x}, \mathbf{w}) - P(K_4; \hat{H}_3; \mathbf{x}, \mathbf{w}) - P(K_4; \hat{H}_4; \mathbf{x}, \mathbf{w}) + P(K_4; \hat{H}_5; \mathbf{x}, \mathbf{w}) \\ P(K_4; \hat{H}_3; \mathbf{x}, \mathbf{w}) - P(K_4; \hat{H}_5; \mathbf{x}, \mathbf{w}) \\ P(K_4; \hat{H}_4; \mathbf{x}, \mathbf{w}) - P(K_4; \hat{H}_5; \mathbf{x}, \mathbf{w}) \\ P(K_4; \hat{H}_5; \mathbf{x}, \mathbf{w}) \end{bmatrix} \\
&= \begin{bmatrix} 0 \\ 0 \\ x_1x_2w_2 + x_1x_3w_2 + x_1x_4w_2 + x_2x_3w_2 + x_2x_4w_2 + x_3x_4w_2 + 3w_2^2 \\ 0 \\ x_1x_2x_3x_4 \end{bmatrix}.
\end{aligned} \tag{8}$$

From (8), it finally follows that $P(K_4; \hat{H}_1; \mathbf{x}, \mathbf{w}) = P(K_4; \hat{H}_2; \mathbf{x}, \mathbf{w}) = P(K_4; \hat{H}_4; \mathbf{x}, \mathbf{w}) = 0$, $P(K_4; \hat{H}_1; \mathbf{x}, \mathbf{w}) = x_1x_2w_2 + x_1x_3w_2 + x_1x_4w_2 + x_2x_3w_2 + x_2x_4w_2 + x_3x_4w_2 + 3w_2^2$, and $P(K_4; \hat{H}_1; \mathbf{x}, \mathbf{w}) = x_1x_2x_3x_4$, which completes our computation. The sum of all thus obtained symmetry-specific polynomials $F(K_4; \hat{H}_j; \mathbf{x}, \mathbf{w})$ equals the R.H.S. of (6) in our Part I.

The above example illustrates how the symmetry-specific polynomials are calculated through symmetry-reduced ones, but not yet how we can compute the latter ones and, more so, symmetry-restricted polynomials which take into account only symmetry-nonequivalent covers.

2.2 Using differential operators to calculate F-polynomials

The topic of differential operators applied to manipulations with graph polynomials was already briefly discussed above (see (7) in Part I and [16–18]). However, in this subsection the same form of differential operator earlier used in (7) of Part I is now employed for modified purposes. Note that the differential operator in (7) of Part I removed the vertex variables not associated with the components f of an F-cover C, whereas in this subsection, we associate this same operator form to eliminate only

variables that exactly pertain to the vertices of respective components f of C. Apparently, from the standpoint of differentiation, there is no difference whatever between the two cases. In other words, we use the following working interpretation of the operator that represents a connected subgraph $\mathsf{f} \in F$;

$$D(\mathsf{f}) := w_{\mathsf{f}} \frac{\partial^s}{\partial x_1 \partial x_2 \cdots \partial x_s} \equiv w_{\mathsf{f}} \partial_1 \partial_2 \cdots \partial_s, \qquad x_i \in V(\mathsf{f}) \quad (1 \le i \le s = |V(\mathsf{f})|;\ \mathsf{f} \in F(G)), \tag{9}$$

where w_{f} is an arbitrary multiplicative weight independent of indeterminates x_i, and where we have introduced abbreviations $\partial_i \equiv \partial/\partial x_i$.

Recall that the product $D_1 \cdot D_2$ of two differential operators in n variables is defined as

$$D_1 \cdot D_2 = w_1 \partial_1^{\beta_1} \partial_2^{\beta_2} \cdots \partial_n^{\beta_n} \cdot w_2 \partial_1^{\gamma_1} \partial_2^{\gamma_2} \cdots \partial_n^{\gamma_n} = w_1 w_2 \partial_1^{\beta_1+\gamma_1} \partial_2^{\beta_2+\gamma_2} \cdots \partial_n^{\beta_n+\gamma_n}, \tag{10}$$

where superscripts β_i and γ_i $(1 \le i \le n)$ are arbitrary nonnegative integers. The set D of all such differential operators generates a commutative and associative algebra D of weighted differential operators in many variables, with a zero $\hat{0}$ and unit $\hat{1}$, over the field W of weight coefficients, such that

(i) under multiplication, D (without 0) forms a semigroup, with identity $\hat{1}$;
(ii) D (with 0) spans a vector space over W.

We say that D is generated by the n derivatives $\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}$ and write $\mathsf{D} = \langle \partial_1, \partial_2, \ldots, \partial_n \rangle$. This simply allows the possibility of addition and multiplication of the differential operators (9) including $\hat{0}$ & $\hat{1}$, with weight coefficients from W. Note that the operator $\hat{0}$ can in most cases be replaced by 0, but a similar substitution of $1 \in \mathsf{W}$ for $\hat{1}$ cannot generally be done except for special cases with $\hat{1}$ standing to the left of D, because for any differential operator $D \in \mathsf{D}$ we have $1D = D$, whereas or $D1 = 0$ (since the differentiation of a constant always gives 0). Just this fact was not properly mentioned in [16–18], where correct final results were in some places accompanied with an incorrect notation 1 instead of the needed $\hat{1}$. See an illustrative example (15) later.

Following De Bruijn's manipulations with Pólya's cycle indices [6], differential operators have been employed for derivation of F-polynomials [16–18], including the *even-subgraph polynomial* $Evn(G; w)$ for the family F of all Eulerian subgraphs, of G, having all vertex degrees even [16]; the characteristic polynomial $\phi^-(G; \mathbf{x})$; the permanental polynomial $\phi^+(G; \mathbf{x})$ (both for the family F of all edges and proper cycles of G); and the matching polynomials $\alpha^-(G; \mathbf{x})$ & $\alpha^+(G; \mathbf{x})$ [17,18]. For $Evn(G; w)$, it was demonstrated [16] that

$$Evn(G; w) = \left\{ \left[\prod_{\substack{\{i,j\} \in E(G) \\ (i<j)}} \left(\hat{1} + w \partial_i \partial_j \right) \right] \prod_{i=1}^{n} \cosh(x_i) \right\} \Bigg|_{x_i = 0 \quad (1 \le i \le n)}, \tag{11}$$

where the first product embraces all edges of G; and $\cosh(x) = (e^x + e^{-x})/2$ is the hyperbolic cosine. As is well known, this yields the partition function of the Ising problem. Though a general version $Evn(G; \mathbf{x}, \mathbf{w})$ of the even-subgraph polynomial is the F-polynomial, its simplified form $Evn(G; w)$ in one variable w, as in (11), is merely the generating function of even subgraphs of a graph G, whose coefficient of w^j is just the number of j-edge even subgraphs of G. The general form also assures the same enumeration if one employs, as components of the vector $\mathbf{w}$, the indeterminates w_j $(1 \le j \le m)$ of weights of respective components $\mathsf{f} \in F$ with exactly j edges.

Thus, the canonical form of an F-polynomial is not generally a linear function in all its variables; however, it is always so in part—namely, in the variables x_i $(1 \le i \le n)$. In mathematics, a polynomial is called a *multiaffine polynomial* if it is of degree 1 in each variable (say, x_i). The (partial) multiaffinity of the F-polynomials in the x_i $(1 \le i \le n)$ plays a crucial role in our differential-operator method [17,18] for an analytic generation of polynomials.

Rosenfeld and Gutman [17,18] obtained the following result (initially formulated for the characteristic, permanental, and matching polynomials but holding true for all F-polynomials):

Theorem 1 *Let $F(G) = \{\mathsf{f}_1, \mathsf{f}_2, \ldots, \mathsf{f}_{|F|}\}$ be a family of connected subgraphs of a graph G, with weights w_f $(\mathsf{f} \in F)$ and associated differential operators $D(\mathsf{f})$, defined in (9). Then*

$$F(G; \mathbf{x}, \mathbf{w}) = \left[\prod_{\mathsf{f} \in F(G)} \left(\hat{1} + w_\mathsf{f} D(\mathsf{f}) \right) \right] \prod_{i=1}^{n} x_i . \tag{12}$$

Proof Apparently, to every 'correct' F-cover in (12), consisting of disjoint components f, there corresponds the product of differential operators containing just the first derivative with respect to each variable used and so contributes to the L.H.S. of (12). On the R.H.S., every product forming an 'incorrect' F-cover must contain overlapping components f, with consequent derivatives of higher-than-first order. Since $\partial^s x_i / \partial x_i^s = 0$ for $s \ge 2$, the 'incorrect' covers do not contribute, leaving only the 'correct', whence the proof is completed. □

Now, we recollect our previous example (6) in Part I and try to reproduce the same result using Theorem 2. Amongst all $2^4 = 16$ differential operators in variables x_1, x_2, x_3, x_4 which occur, only a subset correspond to 'correct' F-covers, Maple or like computational program packages prove useful. As an example:

$$\begin{aligned} M(K_4; \mathbf{x}, \mathbf{w}) = & \left[\left(\hat{1} + w_2 \partial_1 \partial_2 \right) \cdot \left(\hat{1} + w_2 \partial_1 \partial_3 \right) \cdot \left(\hat{1} + w_2 \partial_1 \partial_4 \right) \cdot \right. \\ & \left. \times \left(\hat{1} + w_2 \partial_2 \partial_3 \right) \cdot \left(\hat{1} + w_2 \partial_2 \partial_4 \right) \cdot \left(\hat{1} + w_2 \partial_3 \partial_4 \right) \right] \prod_{i=1}^{4} x_i \\ = & \left[\hat{1} + w_2 \partial_3 \partial_4 + w_2 \partial_2 \partial_4 + w_2 \partial_2 \partial_3 + w_2 \partial_1 \partial_4 \right. \end{aligned} \tag{13}$$

$$+w_2\partial_1\partial_3 + w_2\partial_1\partial_2 + 3w_2^2\partial_1\partial_2\partial_3\partial_4\Big]\prod_{i=1}^{4}$$
$$x_i = x_1x_2x_3x_4 + x_1x_2w_2 + x_1x_3w_2 + x_1x_4w_2 + x_2x_3w_2 + x_2x_4w_2$$
$$+x_3x_4w_2 + 3w_2^2,$$

where the final result is indeed identical to the R.H.S. of (6) in Part I. Again note that the unit $\hat{1}$ of the differential-operator ring D is not an "unnecessary pedantic notion". If 1 were substituted for $\hat{1}$ in (13), one would not obtain the same result; and even the very associativity of multiplication of combined operators in parentheses would be lost. For instance,

$$\left[\left(\hat{1} + w_2\partial_1\partial_2\right)\left(\hat{1} + w_2\partial_3\partial_4\right)\right]x_1x_2x_3x_4 = \left[\hat{1} + w_2\partial_1\partial_2 + w_2\partial_3\partial_4 + w_2^2\partial_1\partial_2\partial_3\partial_4\right]$$
$$\times x_1x_2x_3x_4 = x_1x_2x_3x_4 + x_3x_4w_2 + x_1x_2w_2 + w_2^2,$$

since $w_2\partial_1\partial_2\hat{1} = w_2\partial_1\partial_2$, whereas, if $\hat{1}$ is replaced by 1, then the final term $x_3x_4w_2$ is missing, because $w_2\partial_1\partial_2 1 = 0$. Further, we recommend exploitation of Maple. Note that due to the associativity of the binary multiplicative operation $(\cdot)$, the result displayed by (13) can also be obtained using a successful application of all operators $(\hat{1} + w_2\partial_i\partial_j)$ $(1 \le i, j \le n)$ first to $\prod_{i=1}^{4} x_i$ and, then, each time, to the precedent (intermediate) result. Calculations with Maple give an automated procedure replacing a successive manual one in (13):

maple;
$f_0 := x_1 \cdot x_2 \cdot x_3 \cdot x_4$;
$f_1 := f_0 + diff(f_0, x_1, x_2)$;
(where f_0 is a function $f_0(x_1, x_2)$ in variables x_1 and x_2)
$f_2 := f_1 + diff(f_1, x_1, x_3)$;
$f_3 := f_2 + diff(f_2, x_1, x_4)$;
$f_4 := f_3 + diff(f_3, x_2, x_3)$;
$f_5 := f_4 + diff(f_4, x_2, x_4)$;
$f_6 := f_5 + diff(f_5, x_3, x_4)$;
end;
$M(K_4; \mathbf{x}, \mathbf{w}) = f_6$.

A "trick" with a substitution for $\hat{1}$ appears in a modified version of Theorem 1:

Corollary 1.1 *Let $F(G) = \{\mathsf{f}_1, \mathsf{f}_2, \ldots, \mathsf{f}_{|F|}\}$ be a family of connected subgraphs of a graph G, with weights w_{f} $(\mathsf{f} \in F)$ and associated differential operators $D(\mathsf{f})$, defined in (9). Besides, let ξ be an x_i-independent $(1 \le i \le n)$ variable. Then*

$$F(G; \mathbf{x}; \mathbf{w}) = \left\{\left[\prod_{\mathsf{f}\in F(G)}\left(\frac{\partial}{\partial\xi} + w_{\mathsf{f}}D(\mathsf{f})\right)\right]e^{\xi}\prod_{i=1}^{n}x_i\right\}e^{-\xi}$$

$$= \left\{ \left[\prod_{\mathsf{f} \in F(G)} \left(\frac{\partial}{\partial \xi} + w_{\mathsf{f}} D(\mathsf{f}) \right) \right] e^{\xi} \prod_{i=1}^{n} x_i \right\} \Bigg|_{\xi=0}, \tag{14}$$

where the first product embraces all connected subgraphs $\mathsf{f} \in F(G)$.

Proof Evidently, for all nonnegative integers p, $\frac{\partial^p}{\partial \xi^p} e^{\xi} = e^{\xi}$, which proves the first equality. The second follows from the fact that $e^{\xi}\big|_{\xi=0} = e^0 = 1$. This gives the overall proof. □

Corollary 1.1 does not involve $\hat{1}$, as such, and employs different methods of representing the same operations, as now can be directly programmed for symbolic computations. But from an analytical point of view, an elegant way to calculate the F-polynomials uses differential operators in exponential functions $e^{w_{\mathsf{f}} D} = \hat{1} + \sum_{n=1}^{\infty} \frac{1}{n!} w_{\mathsf{f}}^n D^n$. Then (see [17,18]):

Corollary 1.2 *Let* $F = \{\mathsf{f}_1, \mathsf{f}_2, \ldots, \mathsf{f}_{|F|}\}$ *be a family of connected subgraphs of a graph* G*, with weights* w_{f} $(\mathsf{f} \in F)$ *and associated differential operators* $D(\mathsf{f})$*, defined in (9). Then*

$$F(G; \mathbf{x}; \mathbf{w}) = \left[\exp \left(\sum_{\mathsf{f} \in F(G)} w_{\mathsf{f}} D(\mathsf{f}) \right) \right] \prod_{i=1}^{n} x_i, \tag{15}$$

where the summation ranges over all connected subgraphs $\mathsf{f} \in F$.

Proof Obviously, $\left[\exp \left(\sum_{\mathsf{f} \in F(G)} w_{\mathsf{f}} D(\mathsf{f}) \right) \right] = \left[\prod_{\mathsf{f} \in F(G)} \exp \left(w_{\mathsf{f}} D(\mathsf{f}) \right) \right]$. Since $\left[\exp \left(w_{\mathsf{f}} D(\mathsf{f}) \right) \right] \prod_{i=1}^{n} x_i = \left[\hat{1} + w_{\mathsf{f}} D(\mathsf{f}) \right] \prod_{i=1}^{n} x_i$, we have the proof. □

Theorem 1 and Corollary 1.2 are of use in different ways:

(*) for the study of interrelations among different F-polynomials (which is also one of the main tasks in Farrell's program of investigation;

(**) for the calculation of a specific F-polynomial of one graph through that of another graph;

(***) for derivations of recursion formulae for F-polynomials, and

(****) for identification of a family F of connected subgraphs f of a graph G using the associated F-polynomial $F(G; \mathbf{x}, \mathbf{w})$, as is due to the invertibility of the exponential operator $\left[\exp \left(\sum_{\mathsf{f} \in F(G)} w_{\mathsf{f}} D(\mathsf{f}) \right) \right]$ in the ring D.

Now, recall the set $O(H) = H \backslash\backslash X = \{X_1(H), X_2(H), \ldots, X_s(H)\}$ of orbits induced by a finite (not necessarily closed) subgroup $H \subseteq A$ on a nonempty finite set X. To an orbit $X_j(H) = \{x_{j_1}, x_{j_2}, \ldots, x_{j_p}\}$ $(1 \leq j \leq s; p = p(H) = |X_j(H)|)$, associate the useful differential operator

$$D(X_j(H)) := y_p \partial_{j_1} \partial_{j_2} \cdots \partial_{j_p}, \tag{16}$$

where y_p is a new weight-indeterminate indicating a vertex orbit of cardinality p.

Also, the notion of orbits applies to other than vertices. Given an $f \in F(G)$, an (F-) orbit $X_i(H)$ consists of $f \in F(G)$ all of which are equivalent under $H \subseteq \mathrm{Aut}G$ and the set of such orbits is denoted $\mathcal{F}_H = H\backslash\backslash F = \{F_1(H), F_2(H), \ldots, F_t(H)\}$. We remind the reader that, throughout this paper, $F(G)$ contains full isomorphism classes of subgraphs f of G. Call an orbit $F_k(H) \in \mathcal{F}_H$ $(1 \le k \le t)$ a *free orbit* whenever for each $f \in F_k(H)$ the image $g\mathsf{f}$ of f under every permutation $g \in H$ either has a zero intersection with f or fixes all points of f (call it a *nonfree orbit* otherwise). The weight $w_{F_k}(H)$ $(1 \le k \le t;\ H \subseteq A)$ of a free orbit $F_k(H)$ includes the product of the weights w_{f} of all subgraphs f belonging to it; since these weights are the same for all $q_k = |F_k(H)|$ symmetry-equivalent subgraphs $\mathsf{f} \in F_k(H)$, we have $w_{F_k(H)} = z_{r_k(H)} w_{\mathsf{f}}^{q_k}(H)$, where $r_k(H) = q_k|V(\mathsf{f})|$, or a total number of vertices, of X, covered by a free orbit $F_k(H)$ of connected subgraphs $\mathsf{f} \in F_k(H)$ (the latter version can also be applied to a nonfree orbit), and a new added, weight-indeterminate z_u indicates an orbit $F_k(H)$ of connected subgraphs $\mathsf{f} \in \mathcal{F}_H$ covering exactly $u = r_k$ vertices of X.

Generalizing (9) and (16), we associate to an orbit $F_k(H)$ $(1 \le k \le t)$ the following differential operator

$$D\left(F_k(H)\right) := \begin{cases} z_{r_k} w_{\mathsf{f}}^{q_k} \partial_1 \partial_2 \cdots \partial_l & \text{if } F_k(H) \text{ is free} \quad [\{x_1, x_2, \ldots, x_l\} = V\left(F_k(H)\right)]; \\ \hat{0}, & \text{otherwise.} \end{cases} \tag{17}$$

In our manipulations, we often use a reduced version $D\left(F_k(H)\right) = z_u \partial_1 \partial_2 \cdots \partial_l$ without the usual weight $w_{\mathsf{f}}^{q_k}$.

For further practical applications, we use symmetry-restricted polynomials $P(G; H; \mathbf{y}, \mathbf{z})$ with new variables y_p and z_u. Here, it is worth mentioning that the topic of graph polynomials can be regarded as a part of a more general one of *hypergraph polynomials*. In our case, we have a hypergraph $Hyp(X; E^*)$ with the same vertex set X and the set E^* of hyperedges which are simply orbits $X_i(H)$ of vertices and free orbits $F_j(H)$ of edges induced by a subgroup $H \subseteq A$, or $E^* = O(H) \cup \mathcal{F}_H$. The role of the family F^* of 'connected hypergraphs' can be played by the hyperedge set E^*; in such a case, we might talk of the *hypermatching polynomial of a hypergraph* Hyp or, by some abuse of language, even the *hypermatching polynomial of a graph* G. Additionally, note that the adjective "free" used above is a facultative provision for edge orbits included in F^*, since nonfree orbits correspond to a zero operator $\hat{0}$ in (17). Notice also that hypergraphs can model multiparticle interactions in a molecule, while usual graphs can be viewed to describe only binary interactions between atoms (or orbitals).

This subsection's final, practical result is simply a technical mutation of Theorem 1:

Proposition 2 *Let $P(G; H; \mathbf{y}, \mathbf{z})$ be a generalized symmetry-restricted polynomial of a graph G as above. Then*

$$P(G; H; \mathbf{y}, \mathbf{z}) = \left\{ \prod_{X_j \in O(H)} \prod_{F_k \in \mathcal{F}_H} \left[\left(\hat{1} + D(X_j(H))\right) \left(\hat{1} + D(F_k(H))\right) \right] \right\} \prod_{i=1}^{n} x_i \Bigg|_{\substack{x_i = 0 \\ (1 \le i \le n)}}, \tag{18}$$

where the first and the second products embrace all vertex orbits $X_j(H)$ and all (free) edge orbits $F_k(H)$ induced by a subgroup $H \subseteq A$, respectively.

Proof The proof is based on Lemma 1 and is similar to that of Theorem 2. The additional condition $x_i = 0$ $(1 \leq i \leq n)$ is imposed to eliminate all terms containing auxiliary variables x_i which do not enter the polynomial $P(G; H; \mathbf{y}, \mathbf{z})$, by definition. □

Note that since all variables y_p and z_u are associated with 'vertex cardinalities' of respective orbits (of both vertices and edges), all literal terms in the polynomial $P(G; H; \mathbf{y}, \mathbf{z})$ also obey the Rule 1 (of Part I), as is easily seen, provided that one substitutes any third character for both y and z and conserves all subscripts. Awareness of cycle indices is suggestive that this property is further useful for performing our major task—when we use these $P(G; H; \mathbf{y}, \mathbf{z})$ to compute the generalized cycle indicators enumerating substitutional isomers with symmetry restrictions. Thence, we turn in the next subsection to consider these matters.

2.3 Pólya's cycle indicator and its refinements

Without exaggeration, one may say that the works of Redfield [19] and Pólya [1] founded the basis of the modern theory [2–4,11] of enumeration of objects distinguishable under the automorphism group. The main earlier known underlying tool was the Cauchy-Frobenius lemma (often called [20] Burnside's lemma). Pólya utilized this result to derive his celebrated counting theorem introducing a special generating function now called Pólya's cycle index (or indicator) [1]. Although there are powerful methods employing double cosets [21,22] or Burnside's table of marks [13,14], Pólya's cycle index [1] and its refinements have persisted [3,4,10,11,23–25]. Specifically, we adapt herein a combinatorial method [12] which may be called a *double-Pólya approach*, because it applies the classic Pólya approach twice, at two consecutive levels—first, to a closed subgroup $\hat{H} \subseteq A \cong \mathrm{Aut}X$ acting on a basic set X and, then, to its normalizer $N_A(\hat{H})$ acting both on the set $\hat{H}\backslash\backslash X$ of orbits, induced by $\hat{H}$, and on X itself, where $N_A(\hat{H}) \cong \mathrm{Aut}(\hat{H}\backslash\backslash X)$ (as in Theorem 1 in [11] or below). Earlier [11], we called it a *normalizer approach*. Now, we shall consider this subject more thoroughly.

For an arbitrary subgroup $H \subseteq A$, the *normalizer* $N_A(H) := \{g \in A \mid gH = Hg\}$. With respect to combinatorial actions of $N_A(\hat{H})$ on the set $\hat{H}\backslash\backslash X$ of orbits induced by a closed subgroup $\hat{H}$ on the set X, we proved the following (Theorem 1 on p. 115 of [12]):

Theorem 3 *Let $\hat{H}$ be a closed subgroup of A. Then the normalizer $N_A(\hat{H})$ is the maximum subgroup, in A, the elements of which permute the intact orbits of $\hat{H}$ on X.*

We specially emphasize that, in general, Theorem 3 does not work for an arbitrary subgroup H—just for its closure $\hat{H}$. This result was initially known as an empirical observation concerning crystallographic symmetry groups, and the rigorous proof [11] opened an avenue of further applications, including the computation of special generating functions of the number of substitutional isomers in the present work.

Let $A = \mathrm{Aut}X$ be the automorphism (or permutation) group acting on a nonempty finite set X of objects, as above. Pólya [1] showed that *A-equivalence classes of objects*, or *A-orbits*, can be enumerated by weight, by means of the polynomial called the *cycle index* [2–4]:

$$C(A;X) = C(A;X;s_1,s_2,\ldots,s_n) = \frac{1}{|A|}\sum_{g\in A}\prod_{i\,|\,|A|} s_i^{\varsigma_i(\langle g\rangle)}, \tag{19}$$

where $|A|$ is the cardinality of a group A; the s_i are weight-indeterminates; $\varsigma_i(\langle g\rangle)$ is the number of orbits of length i induced by the cyclic group $\langle g\rangle$ generated by an element $g \in A$; the sum runs over all elements of A; and the product is taken over all divisors i of $|A|$. We mention that $\varsigma_i(g)$ a new notation $\varsigma_i(\langle g\rangle)$ is so as to extend the old tradition with just cyclic (1-generator) subgroups, now to deal with more general subgroups $\langle S\rangle$ generated by the members of $S \subseteq A$ (see [11]). Also, a varsigma version "ς" is used in place of the previous usual character "σ". We choose such a connotation, because all literal terms of cycle indicators also obey the Rule 1 of Part I. As already mentioned, just this similarity in properties of literal terms of the F-polynomials of graphs and cycle indices allows extension of the general combinatorial results of [12] to the case of the generating functions under consideration.

Let $K = \{c_1, c_2, \ldots, c_{|K|}\}$ be a set of weight-indeterminates each standing for one of $|K|$ distinct colors. Then, a version of Pólya's counting theorem [1–4,11,23] is:

Theorem 4 *The number of A-equivalence classes of K-colorings of X with a given assortment of K-colors equals the corresponding coefficient of the polynomial*

$$C(A;X;c_1,c_2,\ldots,c_n) = C(A;X;s_1,s_2,\ldots,s_n)\Big|_{s_i=\sum_{t=1}^{|K|}c_t^i \quad (i\,|\,|A|)}. \tag{20}$$

Here, we can turn from coloring individual elements of X to coloring intact $\hat{H}$-orbits (*i.e.*, elements $X(\hat{H})$ of the set $\hat{H}\backslash\backslash X$). The following statement is an elementary corollary of the Theorems 3 and 4 (see Lemma 3 on p. 116 of [10]):

Lemma 5 *The number of A-equivalence classes of K-colorings of $\hat{H}\backslash\backslash X$ with a given assortment of K-colors equals the corresponding coefficient of the polynomial*

$$C(N_A(\hat{H});\hat{H}\backslash\backslash X;c_1,c_2,\ldots,c_n) = \left[\frac{1}{|N_A(\hat{H})|}\sum_{g\in N_A(\hat{H})}\prod_{i\,|\,|N_A(\hat{H})|} s_i^{\varsigma_i(\langle g\rangle)}\right]_{\substack{s_i=\sum_{t=1}^{|K|}c_t^i \\ (i\,|\,|A|)}}. \tag{21}$$

Lemma 5 just symbolizes the Pólya-type approach with consideration of the actions of $N_A(\hat{H})$ on $\hat{H}\backslash\backslash X$. Below, in Theorem 4, we utilize this universality of Pólya's counting theorem for counting equivalence classes of arbitrary objects, disregarding their nature, yet on larger scales.

Apparently, the maximum orbit length realizable in the 'second-level set' $N_A(\hat{H})\backslash\backslash(\hat{H}\backslash\backslash X)$ 'of orbits on orbits' is $b = |N_G(\hat{H})|/|\hat{H}|$. Note that $\hat{H}$ lies in

the kernel of the action of $N_A(\hat{H})$ on $H\backslash\backslash X$, whence we can replace $N_A(\hat{H})$ with $N_A(\hat{H})/\hat{H}$ and, therefore, restrict the summation over the complete normalizer $N_A(\hat{H})$ to that over the left cosets $g\hat{H}$ of $\hat{H}$ in $N_A(\hat{H})$. As a result (see Lemma 4 on p. 116 of [12]):

Lemma 6 *Let $C(N_A(\hat{H}); \hat{H}\backslash\backslash X)$ be the above cycle indicator. Then*

$$C(N_A(\hat{H}); \hat{H}\backslash\backslash X; s_1, s_2, \ldots, s_n) = \frac{1}{b} \sum_{g\hat{H}\in N_A(\hat{H})/\hat{H}} \prod_{i=1}^{|H\backslash\backslash X|} s_i^{\varsigma_i(\langle g\hat{H}\rangle)} = \frac{1}{b} \sum_{g\in J} \prod_{i\,|\,b} s_i^{\varsigma_i(\langle g\rangle)}, \tag{22}$$

where the first summation goes over all left cosets of $\hat{H}$ in $N_A(\hat{H})$; $\langle g\hat{H}\rangle$ is the subgroup generated by elements of $g\hat{H}$; the first product is over all divisors of $|H\backslash\backslash X|$; the second summation goes over the members of a transversal J ($|J| = b$) of left cosets gH; and the last product is over all divisors of b.

Evidently, this is a special version of Pólya's counting theorem, for the 'second-level set' $\hat{H}\backslash\backslash X$ and an initial subgroup's normalizer $N_A(\hat{H})$. The transversal J above need not be a subgroup of $N_A(\hat{H})$. Indeed, there may exist no subgroup $H' \cong N_A(\hat{H})/\hat{H}$ in $N_A(\hat{H})$ at all (or there may exist more than one).

Now, each orbit of $\langle g\hat{H}\rangle\backslash\backslash(\hat{H}\backslash\backslash X)$ is the union of complete orbits from $\hat{H}\backslash\backslash X$. Also, in the case of groups, all orbits of the latter set comprising one orbit of the former set, have the same cardinality. Then, one can derive (as in Lemma 5 on p. 118 of [11]):

Lemma 7 *Let $\hat{H}$ ($\hat{H} \subseteq A$) be a closed subgroup of A. The number of A-equivalence classes of $\hat{H}$-invariant K-colorings of X, with a given assortment of colors equals the corresponding coefficient of the generalized cycle index*

$$Q(\hat{H}; X; c_1, c_2, \ldots, c_n) = Q(\hat{H}; X; s_1, s_2, \ldots, s_n)\Big|_{s_i=\sum_{t=1}^{|K|} c_t^i \quad (1\le i\le n)}, \tag{23}$$

where (with J as in Lemma 6)

$$Q(\hat{H}; X; s_1, s_2, \ldots, s_n) := \frac{1}{b} \sum_{g\in J} \prod_{p\,|\,b} \prod_{q\,||\,\hat{H}|} s_{p\cdot q}^{\varsigma_{p\cdot q}(\langle g\hat{H}\rangle)}. \tag{24}$$

A generalization of Pólya's theorem follows (Theorem 6 on p. 118 of [12]):

Theorem 8 *The number of A-equivalence classes of $\hat{H}$-invariant K-colorings of X with a given assortment of K-colors equals the corresponding coefficient of the polynomial*

$$Q(\hat{H}; X; c_1, c_2, \ldots, c_n) = \left[\frac{1}{b} \sum_{g\in J} \prod_{i\,||N_A(\hat{H})|} s_i^{\varsigma_i(\langle g\hat{H}\rangle)}\right]_{s_i=\sum_{t=1}^{|K|} c_t^i \quad (1\le i\le n)}, \tag{25}$$

where

$$\left[\frac{1}{b}\sum_{g\in J}\prod_{i\,|\,|N_A(\hat{H})|} s_i^{\zeta_i(\langle g\hat{H}\rangle)}\right] = Q(\hat{H};X;s_1,s_2,\ldots,s_n). \tag{26}$$

Evidently, setting $\hat{H}=\{e\}$ ($|\{e\}|=1$) in (7) of Part I gives the famous Pólya's counting theorem as an immediate corollary of Theorem 8.

Now, recall that literal monomials (such as $\prod_{i\,|\,b} s_i^{\zeta_i(\langle g\rangle)}$ etc.) in all sorts of cycle indices above indicate a certain distribution of a support set X into orbits $X_1, X_2, \ldots, X_s$. But we consider this distribution into orbits also as an F-cover C, of X, with hyperedges, which are the orbits $X_j(\hat{H})$ induced on X by a closed subgroup $\hat{H}\in A$. However, a monomial is sufficient to represent just the distribution of one set of objects (X or any other). If one simultaneously considers, in one combined problem, several sorts of orbit distributions (say, of sets of vertices, edges, cycles, etc. of a graph), one literal monomial is insufficient, since several F-covers of a support set X then exist for it. Thus, we undoubtedly need a polynomial where every literal term corresponds exactly to a different sort of orbit distribution (or F-cover) while numerical coefficients indicate the numbers of corresponding distributions (F-covers). To deal with this, we need to address further the polynomials $P(G;\hat{H};\mathbf{y},\mathbf{z})$ of Proposition 2. Their application is best demonstrated by the following polynomial extension of the Theorem 8, directed to the case of a simultaneous distribution of several sets:

Proposition 9 *Let $Q(N_A(\hat{H});\hat{H}\backslash\backslash X)$ be the above cycle index. Then*

$$Q(N_A(\hat{H});\hat{H}\backslash\backslash X;\mathbf{y};\mathbf{z}) = \frac{1}{b}\sum_{g\in J} P(\langle g\hat{H}\rangle;\hat{H}\backslash\backslash X;\mathbf{y},\mathbf{z}), \tag{27}$$

where the same 'special' weight-indeterminates, introduced above, are adopted; and the summation ranges over members of a transversal J of the left cosets $g\hat{H}$ in $N_A(\hat{H})$.

Note that, even if $\hat{H}$ in (27) is a closed subgroup, $\langle g\hat{H}\rangle$ might not be closed. Also, our 'polynomial extension' above was employed by Harary and Palmer [4] to count orientations of a graph.

To treat all possible K-colorings of X, we need only all closed subgroups $\hat{H}\subseteq A$. Besides, since all conjugated subgroups have the same cycle index Q, as well as C, we may confine ourselves to a fixed transversal $\mathcal{T}$ of conjugacy classes of closed subgroups.

The symmetry-specific cycle indicators $R(\hat{H};X)$'s which correspond to K-colorings of X (res. $\hat{H}\backslash\backslash X$) for which $\hat{H}$ is exactly the automorphism group are calculated through all needed indicators $Q(\hat{H};X)$'s using the exclusion and inclusion argument and combinatorial incidence functions (ζ- & μ-functions). Direct solution of the corresponding system of simultaneous linear equations for all $R(\hat{H};X)$'s, is possible, as well; see a case in point dealing with substituted benzenes on p. 109–112 of [12]. Let $\mathbf{R}$ (res. $\mathbf{Q}$) be a column vector with components $R_i = F(G;\hat{H}_i;\mathbf{y},\mathbf{z})$ (res. $Q_i = Q(G;\hat{H}_i;\mathbf{y},\mathbf{z})$) $(1\le i\le r)$. Then, the solution of our system of simultaneous linear equations, with a coefficients matrix $\underline{\underline{\zeta}}$, is

$$\mathbf{R} = \underline{\underline{\zeta}}^{-1}\mathbf{Q} = \underline{\underline{\mu}}\mathbf{Q}, \tag{28}$$

as is similar to (6).

At this stage of our exposition, we may turn to solving actual tasks of practical use to chemistry (and perhaps to other fields).

3 Illustrative application

Here, we consider practical applications of the theoretical approaches discussed in preceding sections, beginning with simpler tasks. Problems with more complex molecules may be solved in a similar way using associated information on their symmetry group and lattice of (closed) subgroups. A trigonal prismatic skeleton is considered, with monodentate & bidentate ligands.

Among molecules having only covalent bonds and trigonal prismatic geometry with the symmetry group D_{3h}, one case is prismane C_6H_6. Another case is $W(CH_3)_6$ which however is slightly distorted to C_{3v} symmetry. Among inorganic coordination complexes with a coordination number 6, octahedral symmetry prevails. Instances with trigonal-prismatic symmetry are $Mo(SCHCHS)_3$, tris(cis(-1,2-diphenylene)-1,2-dithiolate)rhenates and molybdates, *e.g.*, $Me_2^{1+}[Re(S_2C_2(C_6H_5)_2)_3]^{2-}$ and $[Ph_4As]_2^{1+}[Mo(S_2C_2(CN)_2)_3]^{2-}$.

Figure 1 displays a fixed numbering of vertices of a trigonal prism which is used hereafter. For further manipulations, we need also to introduce a fixed numeration of edges, *viz.:* $e_1 = \{1, 2\}, e_2 = \{1, 3\}, e_3 = \{1, 4\}, e_4 = \{2, 3\}, e_5 = \{2, 5\}, e_6 = \{3, 6\}, e_7 = \{4, 5\}, e_8 = \{4, 6\}, e_9 = \{5, 6\}$.

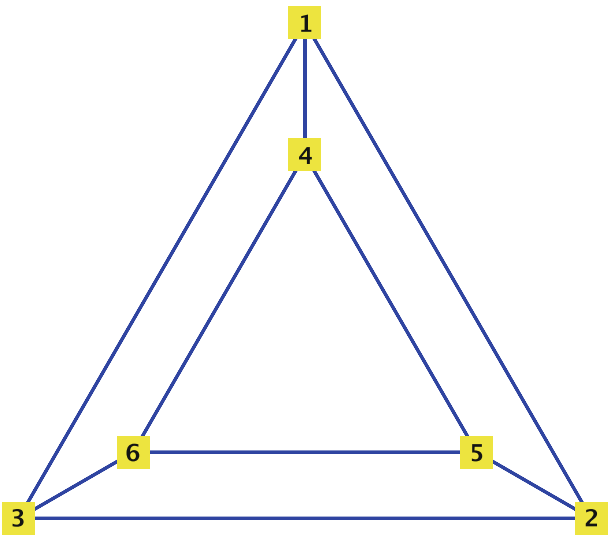

Fig. 1 A graph of the *trigonal* prism

3.1 Structural isomers

The symmetry group D_{3h} is comprised from 12 permutations, viz.:

$$\begin{array}{ll}
\{h_1 = (1)(2)(3)(4)(5)(6) = \left(\begin{smallmatrix}1&2&3&4&5&6\\1&2&3&4&5&6\end{smallmatrix}\right), & h_2 = (1,5)(2,4)(3,6) = \left(\begin{smallmatrix}1&2&3&4&5&6\\5&4&6&2&1&3\end{smallmatrix}\right),\\
h_3 = (1,4)(2,6)(3,5) = \left(\begin{smallmatrix}1&2&3&4&5&6\\4&6&5&1&3&2\end{smallmatrix}\right), & h_4 = (1,6)(2,5)(3,4) = \left(\begin{smallmatrix}1&2&3&4&5&6\\6&5&4&3&2&1\end{smallmatrix}\right),\\
h_5 = (1,2)(3)(4,5)(6) = \left(\begin{smallmatrix}1&2&3&4&5&6\\2&1&3&5&4&6\end{smallmatrix}\right), & h_6 = (1)(2,3)(4)(5,6) = \left(\begin{smallmatrix}1&2&3&4&5&6\\1&3&2&4&6&5\end{smallmatrix}\right),\\
h_7 = (1,3)(2)(4,6)(5) = \left(\begin{smallmatrix}1&2&3&4&5&6\\3&2&1&6&5&4\end{smallmatrix}\right), & h_8 = (1,2,3)(4,5,6) = \left(\begin{smallmatrix}1&2&3&4&5&6\\2&3&1&5&6&4\end{smallmatrix}\right),\\
h_9 = (1,3,2)(4,6,5) = \left(\begin{smallmatrix}1&2&3&4&5&6\\3&1&2&6&4&5\end{smallmatrix}\right), & h_{10} = (1,4)(2,5)(3,6) = \left(\begin{smallmatrix}1&2&3&4&5&6\\4&5&6&1&2&3\end{smallmatrix}\right),\\
h_{11} = (1,5,3,4,2,6) = \left(\begin{smallmatrix}1&2&3&4&5&6\\5&6&4&2&3&1\end{smallmatrix}\right), & h_{12} = (1,6,2,4,3,5) = \left(\begin{smallmatrix}1&2&3&4&5&6\\6&4&5&3&1&2\end{smallmatrix}\right)\}.
\end{array}$$

There are 10 pairwise nonconjugated subgroups: C_1 of order 1, C_2', C_s, & C_s' of order 2; C_3 of order 3; C_{2v} of order 4; D_3, S_3, & C_{3v} of order 6, and D_{3h} itself of order 12. In our case, closed subgroups are C_1, C_2', C_s, C_s', C_{2v}', C_{3v}, & D_{3h}. The other 3 subgroups are not closed: C_3 is coorbital with its closure C_{3v}, while D_3 & S_3 are coorbital with D_{3h}. But because C_3 & S_3 are formally involved in calculating the generalized indicator $Q(N_{D_{3h}}(\hat{C}_1); \hat{C}_1\backslash\backslash X; \mathbf{y}; \mathbf{z}) = Q(D_{3h}; C_1\backslash\backslash X; \mathbf{y}; \mathbf{z})$, these 2 nonclosed subgroups also arise. Therefore, as yet, there is no special economy of time if we exclude the remaining subgroup D_3—at least when we represent needed subgroups of D_{3h} by permutations. Nevertheless, in general, a certain economy may be achieved when it is further needed to calculate the $\zeta-$ and Möbius functions (though herein, we have but a modest economy with 7×7 matrices vs. 10×10 ones). Choosing the closed-subgroup option, we should, however, note that one may also employ the entire lattice of all subgroups while applying the inclusion-exclusion procedure for calculation of these functions; especially, if for some reason it is difficult to find closed subgroups quickly. This might take place, say, when a complex mixture of polydentate ligands arises, because ligands with distinct numbers of ligating sites induce in general different subsets of closed subgroups, and one must then find their overall covering subset. Thus, which option is chosen is to a certain degree dependent on specific circumstances and preferences of the user.

Now, the 10 subgroups of $A = D_{3h}$ are:

$$\begin{aligned}
H_1 &= C_1 = \{h_1\},\\
H_2 &= C_2' = \{h_1, h_2\},\\
H_3 &= C_s = \{h_1, h_{10}\},\\
H_4 &= C_s' = \{h_1, h_5\},\\
H_5 &= C_3 = \{h_1, h_8, h_9\} = \langle h_8\rangle,\\
H_6 &= C_{2v}' = \{h_1, h_2, h_5, h_{10}\} = \langle h_2, h_6\rangle,\\
H_7 &= D_3 = \{h_1, h_2, h_3, h_4, h_8, h_9\} = \langle h_2, h_8\rangle,\\
H_8 &= S_3 = \{h_1, h_8, h_9, h_{10}, h_{11}, h_{12}\} = \langle h_{11}\rangle,\\
H_9 &= C_{3v} = \{h_1, h_5, h_6, h_7, h_8, h_9\} = \langle h_5, h_8\rangle,\\
H_{10} &= D_{3h} = \{h_1, h_2, h_3, h_4, h_5, h_6, h_7, h_8, h_9, h_{10}\} = \langle h_2, h_{11}\rangle,
\end{aligned}$$

where $\langle \cdots \rangle$ denotes the (sub)group generated from a respective set of generators (which are written within the brackets).

The next step is to determine orbits induced by all 10 subgroups of $A = D_{3h}$ on vertices and edges of the triangular prism (in Fig. 1) and write down all differential operators representing these orbits in our approach. The orbits are:

$$
\begin{aligned}
&H_1\backslash\backslash V = \{\{1\},\{2\},\{3\},\{4\},\{5\},\{6\}\}\&\\
&H_1\backslash\backslash E = \{\{1\},\{2\},\{3\},\{4\},\{5\},\{6\},\{7\},\{8\},\{9\}\};\\
&H_2\backslash\backslash V = \{\{1,5\},\{2,4\},\{3,6\}\}\&H_2\backslash\backslash E = \{\{1,7\},\{2,9\},\{3,5\},\{4,8\},\{6\}\};\\
&H_3\backslash\backslash V = \{\{1,4\},\{2,5\},\{3,6\}\}\&H_3\backslash\backslash E = \{\{1,7\},\{2,8\},\{3\},\{4,9\},\{5\},\{6\}\};\\
&H_4\backslash\backslash V = \{\{1,2\},\{3\},\{4,5\},\{6\}\}\&H_4\backslash\backslash E = \{\{1\},\underline{\{2,4\}},\{3,5\},\{6\},\{7\},\underline{\{8,9\}}\};\\
&H_5\backslash\backslash V = \{\{1,2,3\},\{4,5,6\}\}\&H_5\backslash\backslash E = \underline{\{1,2,4\}},\underline{\{3,5,6\}},\underline{\{7,8,9\}};\\
&H_6\backslash\backslash V = \{\{1,2,4,5\},\{3,6\}\}\&H_6\backslash\backslash E = \{\{1,7\},\underline{\{2,4,8,9\}},\{3,5\},\{6\}\};\\
&H_7\backslash\backslash V = \{\{1,2,3,4,5,6\}\}\&H_7\backslash\backslash E = \{\underline{\{1,2,4,7,8,9\}},\{3,5,6\}\};\\
&H_8\backslash\backslash V = \{\{1,2,3,4,5,6\}\}\&H_8\backslash\backslash E = \{\underline{\{1,2,4,7,8,9\}},\{3,5,6\}\};\\
&H_9\backslash\backslash V = \{\{1,2,3\},\{4,5,6\}\}\&H_9\backslash\backslash E = \{\underline{\{1,2,4\}},\{3,5,6\},\underline{\{7,8,9\}}\};\\
&H_{10}\backslash\backslash V = \{\{1,2,3,4,5,6\}\}\&H_{10}\backslash\backslash E = \{\underline{\{1,2,4,7,8,9\}},\{3,5,6\}\},
\end{aligned}
$$

where the numbers j and k substitute for respective vertices v_j and edges e_k, and the underlining indicates nonfree orbits (containing edges with common vertices, and which are not used in construction of differential operators representing orbits, as below).

Now, we give differential operators, with weight multipliers y_s representing vertex orbits, and with weight multipliers z_t representing edge orbits, where subscripts s and t indicate the number of vertices in an orbit (or ligated sites in a molecule). Again, the index t thus indicates a double number of edges in an orbit, rather than that number itself. Moreover, recall that the subscript of variable x_i indicates only the number attached to a vertex which is included in a respective vertex orbit or to that which is incident to a certain edge in an edge orbit—this subscript does not indicate the ordinal number of an edge (even if involved in an operator representing an edge orbit)!

$$
\begin{aligned}
H_1 &= C_1 : y_1\partial_1, y_1\partial_2, y_1\partial_3, y_1\partial_4, y_1\partial_5, y_1\partial_6, z_2\partial_1\partial_2, z_2\partial_1\partial_3, z_2\partial_1\partial_4, z_2\partial_2\partial_3, z_2\partial_2\partial_5,\\
&\quad z_2\partial_3\partial_6, z_2\partial_4\partial_5, z_2\partial_4\partial_6, z_2\partial_5\partial_6;\\
H_2 &= C_2' : y_2\partial_1\partial_5, y_2\partial_2\partial_4, y_2\partial_3\partial_6, z_4\partial_1\partial_2\partial_4\partial_5, z_4\partial_1\partial_3\partial_5\partial x_6, z_4\partial_2\partial_3\partial_4\partial_6, z_2\partial_3\partial_6;\\
H_3 &= C_s : y_2\partial_1\partial_4, y_2\partial_2\partial_5, y_2\partial_3\partial_6, z_4\partial_1\partial_2\partial_4\partial_5, z_4\partial_1\partial_3\partial_4\partial_6, z_2\partial_1\partial_4, z_4\partial_2\partial_3\partial_5\partial_6, z_2\partial_2\partial_5, z_2\partial_3\partial_6;\\
H_4 &= C_s' : y_2\partial_1\partial_2, y_1\partial_3, y_2\partial_4\partial_5, y_1\partial_6, z_2\partial_1\partial_2, z_4\partial_1\partial_2\partial_4\partial_5, z_2\partial_3\partial_6, z_2\partial_4\partial_5;\\
H_5 &= C_3 : y_3\partial_1\partial_2\partial_3, y_3\partial_4\partial_5\partial_6, z_6\partial_1\partial_2\partial_3\partial_4\partial_5\partial_6;\\
H_6 &= C_{2v}' : y_4\partial_1\partial_2\partial_4\partial_5, y_2\partial_3\partial_6, z_4\partial_1\partial_2\partial_4\partial_5, z_4\partial_1\partial_2\partial_4\partial_5, z_2\partial_3\partial_6;\\
H_7 &= D_3 : y_6\partial_1\partial_2\partial_3\partial_4\partial_5\partial_6, z_6\partial_1\partial_2\partial_3\partial_4\partial_5\partial_6;\\
H_8 &= S_3 : y_6\partial_1\partial_2\partial_3\partial_4\partial_5\partial_6, z_6\partial_1\partial_2\partial_3\partial_4\partial_5\partial_6;\\
H_9 &= D_3 : y_3\partial_1\partial_2\partial_3, y_3\partial_4\partial_5\partial_6, z_6\partial_1\partial_2\partial_3\partial_4\partial_5\partial_6;\\
H_{10} &= D_{3h} : y_6\partial_1\partial_2\partial_3\partial_4\partial_5\partial_6, z_6\partial_1\partial_2\partial_3\partial_4\partial_5\partial_6,
\end{aligned}
$$

where all differential operators are given in the same order as the respective vertex and free-edge orbits listed above.

In order to calculate all symmetry-restricted polynomials $P(G; H; \mathbf{y}, \mathbf{z})$, we use (18), which involves operators $D(X_j(H)) = y_s \partial_{j_1} \partial_{j_2} \cdots \partial_{j_s}$ and $D(F_k(H)) = z_t \partial_{k_1} \partial_{k_2} \cdots \partial_{k_t}$, where $H \subseteq D_{3h}$ (as indicated above). We do not demonstrate here all our successive computations by (19), made with the aid of Maple 14, because of a relatively large size of the expressions in variables y_j and z_t—instead giving final working formulae for the simplest mixture of polydentate ligand involving only one sort of monodentate ligand and only one sort of bidentate ones. These are obtained through the substitutions $y_s = 1 + y^s$ and $z_t = z^t$ ($s \in [1, 6]$) therein (where 1 stands for a pristine molecule without ligand). Apparently, familiar considerations of the Pólya's cycle-index method may be applied here to produce similar generating functions for any other numbers of ligand sorts (just using more weight-indeterminates therein). Our 'simplest-case' polynomials are:

$$
\begin{aligned}
P(D_{3h}; H_1\backslash\backslash V; y, z) &= 1 + 6y + 15y^2 + 20y^3 + 15y^4 + 6y^5 + y^6 + (9 + 36y \\
&\quad + 54y^2 + 36y^3 + 9y^4)z^2 + (18 + 36y + 18y^2)z^4 + 4z^6; \\
P(D_{3h}; H_2\backslash\backslash V; y, z) &= 1 + 3y^2 + 3y^4 + y^6 + (1 + 2y^2 + y^4)z^2 + (4 + 4y^2)z^4 + 2z^6; \\
P(D_{3h}; H_3\backslash\backslash V; y, z) &= 1 + 3y^2 + 3y^4 + y^6 + (3 + 6y^2 + 3y^4)z^2 + (6 + 6y^2)z^4 + 4z^6; \\
P(D_{3h}; H_4\backslash\backslash V; y, z) &= 1 + 2y + 3y^2 + 4y^3 + 3y^4 + 2y^5 + y^6 + (3 + 4y + 6y^2 + 4y^3 \\
&\quad + 3y^4)z^2 + (4 + 4y + 4y^2)z^4 + 2z^6; \\
P(D_{3h}; H_5\backslash\backslash V; y, z) &= 1 + 2y^3 + y^6 + z^6; \\
P(D_{3h}; H_6\backslash\backslash V; y, z) &= 1 + y^2 + y^4 + y^6 + (1 + y^4)z^2 + (2 + 2y^2)z^4 + 2z^6; \\
P(D_{3h}; H_7\backslash\backslash V; y, z) &= 1 + y^6 + z^6; \\
P(D_{3h}; H_8\backslash\backslash V; y, z) &= 1 + y^6 + z^6; \\
P(D_{3h}; H_9\backslash\backslash V; y, z) &= 1 + 2y^3 + y^6 + z^6; \\
P(D_{3h}; H_{10}\backslash\backslash V; y, z) &= 1 + y^6 + z^6,
\end{aligned}
$$

where the powers of both y and z indicate the number of ligated sites (rather than the numbers of ligands, in the latter case). Note that $P(D_{3h}; H_1\backslash\backslash V; 0, z)$ is the matching-enumeration polynomial of the prism.

In order to proceed, we first determine the normalizers $N_{D_{3h}}(H_j)$ of subgroups $H_j \subseteq D_{3h}$, then, find their right (res. left) cosets $H_j g$ in the corresponding normalizers, and, further, calculate (sub)groups $\langle H_j g \rangle$ for all such cosets $H_j g$ of every subgroup H_j. Note that Maple has special packages to perform such a task. This information is given here in the following combined form:

$$
\begin{aligned}
N_{D_{3h}}(H_1) &= H_{10} = \langle H_1 h_1 \rangle \cup \langle H_1 h_2 \rangle \cup \langle H_1 h_3 \rangle \cup \langle H_1 h_4 \rangle \cup \langle H_1 h_5 \rangle \cup \langle H_1 h_6 \rangle \cup \langle H_1 h_7 \rangle \\
&\quad \cup H_1 h_8 \rangle \cup \langle H_1 h_9 \rangle \cup \langle H_1 h_{10} \rangle \cup \langle H_1 h_{11} \rangle \cup \langle H_1 h_{12} \rangle = H_1 \cup H_2 \\
&\quad \cup H_2 \cup H_2 \cup H_4 \cup H_4 \cup H_4 \cup H_5 \cup H_5 \cup H_3 \cup H_8 \cup H_8; \\
N_{D_{3h}}(H_2) &= H_6 = \langle H_2 h_1 \rangle \cup \langle H_2 h_5 \rangle = H_2 \cup H_6; \\
N_{D_{3h}}(H_3) &= H_{10} = \langle H_3 h_1 \rangle \cup \langle H_3 h_5 \rangle \cup \langle H_3 h_6 \rangle \cup \langle H_3 h_7 \rangle \cup \langle H_3 h_8 \rangle \cup \langle H_3 h_9 \rangle \\
&= H_3 \cup H_6 \cup H_6 \cup H_6 \cup H_9 \cup H_9; \\
N_{D_{3h}}(H_4) &= H_6 = \langle H_4 h_1 \rangle \cup \langle H_4 h_{10} \rangle = H_4 \cup H_6; \\
N_{D_{3h}}(H_5) &= H_{10} = \langle H_5 h_1 \rangle \cup \langle H_5 h_3 \rangle \cup \langle H_5 h_6 \rangle \cup \langle H_5 h_{10} \rangle = H_5 \cup H_7 \cup H_9 \cup H_8; \\
N_{D_{3h}}(H_6) &= H_6 = \langle H_6 h_1 \rangle = H_6; \\
N_{D_{3h}}(H_7) &= H_{10} = \langle H_7 h_1 \rangle \cup \langle H_7 h_6 \rangle = H_7 \cup H_{10};
\end{aligned}
$$

$$
\begin{aligned}
N_{D_{3h}}(H_8) &= H_{10} = \langle H_8 h_1 \rangle \cup \langle H_8 h_6 \rangle = H_8 \cup H_{10};\\
N_{D_{3h}}(H_9) &= H_{10} = \langle H_9 h_1 \rangle \cup \langle H_9 h_{10} \rangle = H_9 \cup H_{10};\\
N_{D_{3h}}(H_{10}) &= H_{10} = \langle H_{10} h_1 \rangle = H_{10},
\end{aligned}
$$

where the $\langle \hat{H}_j g \rangle$-decomposition of each normalizer determines the subsymmetry-reduced polynomial $Q_j := Q(N_{D_{3h}}(\hat{H}_j); \hat{H}_j \backslash\backslash V; y, z)$ as a linear combination of all respective polynomials $P_j := P(\langle \hat{H}_j g \rangle; \hat{H}_j \backslash\backslash V; y, z)$, done according to (27). Here, recall that the closure $\hat{H}_j$ is used instead of H_j in case if H_j is a nonclosed subgroup $H_j \subset \hat{H}_j$, but this is independent the coset decomposition of normalizers, which is good for either case.

Now, we give the polynomials $Q(N_{D_{3h}}(\hat{H}_j); \hat{H}_j \backslash\backslash V; y, z)$ for all 10 subgroups of D_{3h} (which is in some excess if one wants to use only 7 closed subgroups):

$$
\begin{aligned}
Q_1 &= (1/12)(P_1 + 3P_2 + P_3 + 3P_4 + 2P_5 + 2P_8) = 1 + y + 3y^2 + 3y^3 + 3y^4\\
&\quad + y^5 + y^6 + (2 + 4y + 7y^2 + 4y^3 + 2y^4)z^2 + (4 + 4y + 4y^2)z^4 + 2z^6;\\
Q_2 &= (1/2)(P_2 + P_6) = 1 + 2y^2 + 2y^4 + y^6 + (1 + y^2 + y^4)z^2 + (3 + 3y^2)z^4 + 2z^6;\\
Q_3 &= (1/6)(P_3 + 3P_6 + 2P_8) = 1 + y^2 + y^4 + y^6 + (1 + y^2 + y^4)z^2 + (2 + 2y^2)z^4 + 2z^6;\\
Q_4 &= (1/2)(P_4 + P_6) = 1 + y + 2y^2 + 2y^3 + 2y^4 + y^5 + y^6 + (2 + 2y + 3y^2 + 2y^3\\
&\quad + 2y^4)z^2 + (3 + 2y + 3y^2)z^4 + 2z^6;\\
Q_5 &= (1/4)(P_5 + P_9 + P_7 + P_8) = 1 + y^3 + y^6 + z^6;\\
Q_6 &= (1/1)P_6 = 1 + y^2 + y^4 + y^6 + (1 + y^4)z^2 + (2 + 2y^2)z^4 + 2z^6;\\
Q_7 &= (1/2)(P_7 + P_{10}) = 1 + y^6 + z^6;\\
Q_8 &= (1/2)(P_8 + P_{10}) = 1 + y^6 + z^6;\\
Q_9 &= (1/2)(P_9 + P_{10}) = 1 + y^3 + y^6 + z^6;\\
Q_{10} &= (1/1)P_{10} = 1 + y^6 + z^6,
\end{aligned}
$$

where each denominator of a fractional coefficient is the number of cosets in a respective decomposition of a normalizer. Recall the standard Pólya's cycle-index averaging, here, done over all $|N_{D_{3h}}(H_j)|/|H_j|$ elements of the factor group $N_{D_{3h}}(H_j)/H_j$, which are right cosets $H_j g$.

We know that each symmetry-reduced indicator Q_j above enumerates substitutional isomers whose own automorphism (symmetry) group H obligatorily includes H_j and may in general be larger ($H_j \subseteq H \subseteq A$). In order to calculate symmetry-specific polynomials R_j, enumerating the same isomers but with an exact automorphism group H_j, one should apply the inclusion-exclusion-type procedure, or equivalently the Möbius function. In our case (with 7 closed subgroups), these are both 7×7 matrices. The ζ-function is

$$
\underline{\underline{\zeta}} = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1\\
0 & 1 & 0 & 0 & 1 & 0 & 1\\
0 & 0 & 1 & 0 & 1 & 0 & 1\\
0 & 0 & 0 & 1 & 1 & 1 & 1\\
0 & 0 & 0 & 0 & 1 & 0 & 1\\
0 & 0 & 0 & 0 & 0 & 1 & 1\\
0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix},
$$

where an entry $\zeta_{ij} = 1$ iff $H'_i \subseteq H'_j$ $(1 \le i \le j \le 7)$. In this case, for excluding nonclosed subgroups $H_5 = C_3$, $H_7 = D_3$, and $H_8 = S_3$, we have the following renumbered subgroups: $H'_1 = H_1$, $H'_2 = H_2$, $H'_3 = H_3$, $H'_4 = H_4$, $H'_5 = H_6$, $H'_6 = H_9$, and $H'_7 = H_{10}$. The same correspondence of indices is adopted below, when the prime ($'$) is applied to groups.

The Möbius function is the matrix $\underline{\underline{\mu}} = \underline{\underline{\zeta}}^{-1}$:

$$\underline{\underline{\mu}} = \begin{bmatrix} 1 & -1 & -1 & -1 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

From (29), it follows that $R'_i = \sum \mu_{ij} Q'_j$ $(1 \le i \le j \le 7)$. Hence, we obtain:

$$\begin{aligned}
R_1(C_1) &= R'_1 = Q'_1 - Q'_2 - Q'_3 - Q'_4 + 2Q'_5 = Q_1 - Q_2 - Q_3 - Q_4 + 2Q_6 \\
&= y^3 + (2y + 2y^2 + 2y^3)z^2 + 2yz^4; \\
R_2(C'_2) &= R'_2 = Q'_2 - Q'_5 = Q_2 - Q_6 = y^2 + y^4 + y^2z^2 + (1 + y^2)z^4; \\
R_3(C_s) &= R'_3 = Q'_3 - Q'_5 = Q_3 - Q_6 = y^2z^2; \\
R_4(C'_s) &= R'_4 = Q'_4 - Q'_5 - Q'_6 + Q'_7 = Q_4 - Q_6 - Q_9 + Q_{10} = y + y^2 + y^3 \\
&\quad + y^4 + y^5 + (1 + 2y + 3y^2 + 2y^3 + y^4)z^2 + (1 + 2y + y^2)z^4; \\
R_5(C_3) &= 0; \\
R_6(C'_{2v}) &= R'_5 = Q'_5 - Q'_7 = Q_6 - Q_{10} = y^2 + y^4 + (1 + y^4)z^2 + (2 + 2y^2)z^4 + z^6; \\
R_7(D_3) &= 0; \\
R_8(S_3) &= 0; \\
R_9(C_{3v}) &= R'_6 = Q'_6 - Q'_7 = Q_9 - Q_{10} = y^3; \\
R_{10}(D_{3h}) &= R'_7 = Q'_7 = Q_{10} = 1 + y^6 + z^6,
\end{aligned}$$

where 0s indicate the omission of respective nonclosed subgroups in our inclusion-exclusion procedure. These generating polynomials enumerate substitutional isomers of the prismanes with symmetry exactly corresponding to a respective subgroup $H_j \subseteq D_{3h}$, not distinguishing enantiomers.

3.2 Stereo isomers

In order to enumerate stereomers, we need to perform similar calculations involving the automorphism group D_3 in place of D_{3h}. We have:

$$\begin{aligned}
N_{D_3}(H_1) &= H_7 = \langle H_1 h_1 \rangle \cup \langle H_1 h_2 \rangle \cup \langle H_1 h_3 \rangle \cup \langle H_1 h_4 \rangle \cup \langle H_1 h_8 \rangle \cup \langle H_1 h_9 \rangle \\
&= H_1 \cup H_2 \cup H_2 \cup H_2 \cup H_5 \cup H_5;
\end{aligned}$$

$$
\begin{aligned}
&N_{D_3}(H_2) = H_2 = \langle H_2 h_1\rangle = H_2;\\
&N_{D_3}(H_3) = H_{10} = \langle H_3 h_1\rangle \cup \langle H_3 h_5\rangle \cup \langle H_3 h_6\rangle \cup \langle H_3 h_7\rangle \cup \langle H_3 h_8\rangle \cup \langle H_3 h_9\rangle\\
&\qquad = H_3 \cup H_6 \cup H_6 \cup H_6 \cup H_9 \cup H_9;\\
&N_{D_3}(H_4) = H_6 = \langle H_4 h_1\rangle \cup \langle H_4 h_2\rangle = H_4 \cup H_6;\\
&N_{D_3}(H_5) = H_7 = \langle H_5 h_1\rangle \cup \langle H_5 h_3\rangle = H_5 \cup H_7;\\
&N_{D_3}(H_6) = H_6 = \langle H_6 h_1\rangle = H_6;\\
&N_{D_3}(H_7) = H_7 = \langle H_7 h_1\rangle = H_7;\\
&N_{D_3}(H_8) = H_8 = \langle H_8 h_1\rangle = H_8;\\
&N_{D_3}(H_9) = H_{10} = \langle H_9 h_1\rangle \cup \langle H_9 h_2\rangle = H_9 \cup H_{10};\\
&N_{D_3}(H_{10}) = H_{10} = \langle H_{10} h_1\rangle = H_{10}.
\end{aligned}
$$

For the case of D_3, we label the associated Q_i polynomials by $\bar{Q}_i$ to distinguish them from the Q_i associated with D_{3h}. Then,

$$
\begin{aligned}
\bar{Q}_1 &= (1/6)(P_1 + 3P_2 + 2P_5) = 1 + y + 4y^2 + 4y^3 + 4y^4 + y^5 + y^6\\
&\quad +(2 + 6y + 10y^2 + 6y^3 + 2y^4)z^2 + (5 + 6y + 5y^2)z^4 + 2z^6;\\
\bar{Q}_2 &= (1/1)P_2 = 1 + 3y^2 + 3y^4 + y^6 + (1 + 2y^2 + y^4)z^2 + (4 + 4y^2)z^4 + 2z^6;\\
\bar{Q}_3 &= (1/6)(P_3 + 3P_6 + 2P_9) = 1 + y^2 + y^4 + y^6 + (1 + y^2 + y^4)z^2\\
&\quad +(2 + 2y^2)z^4 + 2z^6;\\
\bar{Q}_4 &= (1/2)(P_4 + P_6) = 1 + y + 2y^2 + 2y^3 + 2y^4 + y^5 + y^6\\
&\quad +(2 + 2y + 3y^2 + 2y^3 + 2y^4)z^2 + (3 + 2y + 3y^2)z^4 + 2z^6;\\
\bar{Q}_5 &= (1/2)(P_5 + P_7) = 1 + y^3 + y^6 + z^6;\\
\bar{Q}_6 &= (1/1)P_6 = 1 + y^2 + y^4 + y^6 + (1 + y^4)z^2 + (2 + 2y^2)z^4 + 2z^6;\\
\bar{Q}_7 &= (1/1)P_7 = 1 + y^6 + z^6;\\
\bar{Q}_8 &= (1/1)P_8 = 1 + y^6 + z^6;\\
\bar{Q}_9 &= (1/2)(P_9 + P_{10}) = 1 + y^3 + y^6 + z^6;\\
\bar{Q}_{10} &= (1/1)P_{10} = 1 + y^6 + z^6.
\end{aligned}
$$

Now, one is to calculate $\bar{R}_j$ polynomials which for D_3 are also denoted by $\bar{R}_j$. This still entails the same ζ- & μ-functions—attaching the bar to capitals R & Q in the expressions deduced for R_j above. Thence, we obtain:

$$
\begin{aligned}
\bar{R}_1(C_1) &= \bar{R}'_1 = \bar{Q}'_1 - \bar{Q}'_2 - \bar{Q}'_3 - \bar{Q}'_4 + 2\bar{Q}'_5 = \bar{Q}_1 - \bar{Q}_2 - \bar{Q}_3 - \bar{Q}_4 + 2\bar{Q}_6\\
&\quad = 2y^3 + (4y + 4y^2 + 4y^3)z^2 + 4yz^4;\\
\bar{R}_2(C'_2) &= \bar{R}'_2 = \bar{Q}'_2 - \bar{Q}'_5 = \bar{Q}_2 - \bar{Q}_6 = 2y^2 + 2y^4 + 2y^2z^2 + (2 + 2y^2)z^4;\\
\bar{R}_3(C_s) &= \bar{R}'_3 = \bar{Q}'_3 - \bar{Q}'_5 = \bar{Q}_3 - \bar{Q}_6 = y^2z^2;\\
\bar{R}_4(C'_s) &= \bar{R}'_4 = \bar{Q}'_4 - \bar{Q}'_5 - \bar{Q}'_6 + \bar{Q}'_7 = \bar{Q}_4 - \bar{Q}_6 - \bar{Q}_9 + \bar{Q}_{10} = y + y^2 + y^3\\
&\quad +y^4 + y^5 + (1 + 2y + 3y^2 + 2y^3 + y^4)z^2 + (1 + 2y + y^2)z^4;\\
\bar{R}_5(C_3) &= 0;
\end{aligned}
$$

$$\bar{R}_6(C'_{2v}) = \bar{R}'_5 = \bar{Q}'_5 - \bar{Q}'_7 = \bar{Q}_6 - \bar{Q}_{10} = y^2 + y^4 + (1 + y^4)z^2 + (2 + 2y^2)z^4 + z^6;$$
$$\bar{R}_7(D_3) = 0;$$
$$\bar{R}_8(S_3) = 0;$$
$$\bar{R}_9(C_{3v}) = \bar{R}'_6 = \bar{Q}'_6 - \bar{Q}'_7 = \bar{Q}_9 - \bar{Q}_{10} = y^3;$$
$$\bar{R}_{10}(D_{3h}) = \bar{R}'_7 = \bar{Q}'_7 = \bar{Q}_{10} = 1 + y^6 + z^6,$$

where again 0s indicate the omission of respective nonclosed subgroups in our inclusion-exclusion procedure.

These R_i enumerate the stereomers of different symmetries. But these may also be resolved into enantiomeric pairs and diastereomers. First, the enantiomeric pairs of different subsymmetries are evidently given as $\bar{R}_i - R_i$, and second, the corresponding diastereomer counts are given as $R_i - S_i$. We find:

$$S_1(C_1) = \bar{R}_1 - R_1 = y^3 + (2y + 2y^2 + 2y^3)z^2 + 2yz^4;$$
$$S_2(C'_2) = \bar{R}_2 - R_2 = y^2 + y^4 + y^2z^2 + (1 + y^2)z^4;$$
$$S_3(C_s) = \bar{R}_3 - R_3 = 0;$$
$$S_4(C'_s) = \bar{R}_4 - R_4 = 0;$$
$$S_5(C_3) = \bar{R}_5 - R_5 = 0;$$
$$S_6(C'_{2v}) = \bar{R}_6 - R_6 = 0;$$
$$S_7(D_3) = \bar{R}_7 - R_7 = 0;$$
$$S_8(S_3) = \bar{R}_8 - R_8 = 0;$$
$$S_9(C_{3v}) = \bar{R}_9 - R_9 = 0;$$
$$S_{10}(D_{3h}) = \bar{R}_{10} - R_{10} = 0,$$

where 0s indicate the nonexistence of enantiomeric substitutional isomers of prismane with the respective subgroups as their automorphism groups.

Finally, symmetry-specific indicators T_j for diastereomers are:

$$T_1(C_1) = R_1 - S_1 = 2R_1 - \bar{R}_1 = 0;$$
$$T_2(C'_2) = R_2 - S_2 = 2R_2 - \bar{R}_2 = 0;$$
$$T_3(C_s) = R_3 - S_3 = 2R_3 - \bar{R}_3 = y^2z^2;$$
$$T_4(C'_s) = R_4 - S_4 = 2R_4 - \bar{R}_4 = y + y^2 + y^3 + y^4 + y^5 + (1 + 2y + 3y^2 + 2y^3 + y^4)z^2 + (1 + 2y + y^2)z^4;$$
$$T_5(C_3) = R_5 - S_5 = 2R_5 - \bar{R}_5 = 0;$$
$$T_6(C'_{2v}) = R_6 - S_6 = 2R_6 - \bar{R}_6 = y^2 + y^4 + (1 + y^4)z^2 + (2 + 2y^2)z^4 + z^6;$$
$$T_7(D_3) = R_7 - S_7 = 2R_7 - \bar{R}_7 = 0;$$
$$T_8(S_3) = R_8 - S_8 = 2R_8 - \bar{R}_8 = 0;$$
$$T_9(C_{3v}) = R_9 - S_9 = 2R_9 - \bar{R}_9 = y^3;$$
$$T_{10}(D_{3h}) = R_{10} - S_{10} = 2R_{10} - \bar{R}_{10} = 1 + y^6 + z^6.$$

The task could also be performed employing the full-size 10×10 matrices for ζ- & μ-functions and all 10 conjugated subgroups of D_{3h}. This allows avoidance of

niceties of closed or nonclosed. To this end, we additionally supplement below such matrices $\underline{\underline{\zeta}}$ & $\underline{\underline{\mu}}$ (prepared with the aid of Maple 14). Viz.:

$$\underline{\underline{\zeta}} = \begin{bmatrix} 1&1&1&1&1&1&1&1&1&1 \\ 0&1&0&0&0&1&1&0&0&1 \\ 0&0&1&0&0&1&0&1&0&1 \\ 0&0&0&1&0&1&0&0&1&1 \\ 0&0&0&0&1&0&1&1&1&1 \\ 0&0&0&0&0&1&0&0&0&1 \\ 0&0&0&0&0&0&1&0&0&1 \\ 0&0&0&0&0&0&0&1&0&1 \\ 0&0&0&0&0&0&0&0&1&1 \\ 0&0&0&0&0&0&0&0&0&1 \end{bmatrix};$$

$$\underline{\underline{\mu}} = \begin{bmatrix} 1&-1&-1&-1&-1&2&1&1&1&-2 \\ 0&1&0&0&0&-1&-1&0&0&1 \\ 0&0&1&0&0&-1&0&-1&0&1 \\ 0&0&0&1&0&-1&0&0&-1&1 \\ 0&0&0&0&1&0&-1&-1&-1&2 \\ 0&0&0&0&0&1&0&0&0&-1 \\ 0&0&0&0&0&0&1&0&0&-1 \\ 0&0&0&0&0&0&0&1&0&-1 \\ 0&0&0&0&0&0&0&0&1&-1 \\ 0&0&0&0&0&0&0&0&0&1 \end{bmatrix}.$$

(A hand repetition of all results using the last two matrices checks.)

4 Discussion

In review, we have adapted the generalized cycle indices from [11] and replaced the monomials in these indices with special generating functions, by analogy with similar procedures described by Harary and Palmer [4]. Other parts of our approach have been borrowed from the theory of the F-polynomials of graphs [5–8,26], the article [12] by Rota and Smith containing the definition of a closed subgroup, our previous papers concerning restrictions imposed on the enumeration of substitutional isomers [27–29], and our experience of earlier applications of differential operators to the derivation of graph polynomials [16–18,26]. The book [30] by Balaban is an additional interesting collection of combinatorial problems arising in chemistry.

Finally, our techniques have been simply illustrated on a sample trigonal prismatic skeleton. These techniques should be much more widely applicable.

In practice, for a complex problem dealing with combinatorial actions of a permutation group A on several sets $(X, Y, \ldots, Z)$ (say, of vertices, edges, *etc.*) at once, one and the same subgroup $H \subseteq A$ may behave as a closed subgroup in actions on one set but not as a closed subgroup on the others. For the overall situation, it is emphasized that a subgroup $H \subseteq A$ must in such a case be considered as a closed subgroup for the entire problem whenever it is a closed subgroup in its actions on at least one of

the mentioned subsets, say X. That is, H is not a closed subgroup if it simultaneously acts as an nonclosed subgroup on all considered sets $X, Y, \ldots, Z$. Disobeying this condition leads to errors in calculations.

During the preparation of this text, we became aware of two papers [31,32] where the symmetry-restricted Tutte polynomial was studied from a different viewpoint. A hybrid of Pólya's cycle index now with the chromatic polynomial was studied. This evidently then falls in the same class of restricted enumerations as our present problem. Possibly, further new results might then result in combination with our present formulation.

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