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Enumeration of substitutional isomers with restrictive mutual positions of ligands: I. Overall counts

Vladimir R. Rosenfeld · Douglas J. Klein

Abstract   We address systematics for the enumeration of substitutional isomers when there is constrained positioning of ligands on a molecular skeleton. One constraint involves 'restrictive ligands' where two of the same kind are forbidden to occupy adjacent sites in a molecular skeleton. This may arise because of steric hindrance, or because of groups which in neighbor proximity react to eliminate one. For instance, no pair of –OH groups attach to the same C atom in a molecular skeleton. In another case, malonic acid residues decarboxylate leaving no more than one decarboxylation in each residue. The enumeration with such restrictive ligands may be addressed via a Polya-theoretic cycle index hybridized with the graph-theoretic independence polynomial (when there is just a single such neighbor-excluding ligand and another which is not), while more generally a hybridization with the chromatic polynomial is needed. Another substitional-isomer constraint involves bidentate ligands, with each ligand-part occupying adjacent sites, and possibly also with additional separate unidentate ligands. Here, the set of all pure & mixed such ligand placements is analytically represented by a 'symmetry-reduced' matching polynomial (which is a hybrid now of the matching polynomial and Polya's cycle index). This result gives the generating function for isomer enumeration, taking into account every possible so-restricted assortment of the employed ligands. Here we make such novel hybridizations (for these and other graphtheoretic polynomials) to deal with such oft-encountered chemical problems, which nevertheless transcend typical earlier unconstrained formulizations.

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: vladimir_rosenfeld@yahoo.com

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

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Further subsymmetry classification & enumerations, along with examples are considered in a further article.

Keywords   Enumeration · Substitutional isomers · Constrained substitution · Symmetry-reduced counting polynomials

1 Introduction

We start with a general introduction to the subject and try to adequately detail basic ideas with a modest selection of references. Our exposition is not sought to be a comprehensive historical (or systematic) survey. A number of selected practical examples in the text illustrate the tasks involved.

Practically all molecules in nature are substitutional isomers of other molecules. This often means that some of them share one and the same core, or *skeleton*, and differ only in their individual sets of substituents, or *ligands*, attached to this skeleton. A diversity of instances can be recalled: substituted benzenes, say, having a benzene ring as a common core; octahedral coordination complexes (as of CO^{2+}) with a fixed central metal ion and a fixed octahedral coordination sphere; bulk crystals built from different atoms but sharing one and the same crystal lattice, in the sense of having isomorphic unit cells; and linear chain molecules of DNA, responsible for all forms of life on Planet Earth; etc. The set S of skeletal sites are locations for the substitution of a finite collection $\mathcal{L}$ of types of ligands. Of the different possible patterns of distributing ligands at the various skeletal sites, some patterns will describe the same chemical compound, such as have certain identical properties. Generally different so equivalent patterns are transformable into one another through some permutation of the ligands and/or skeletal sites. Typically, then the equivalent patterns are those transformable into one another through some permutation group A, and the problem at hand is to enumerate (and characterize) the A-equivalence classes of the patterns.

To this point, we have skeletal and ligand sites and an associated permutation group—and this is the basics of what is involved in Pólya's enumeration theory [1–3]—as well as in Cauchy-Frobenius' [2,3], Redfield's (see [4]), Ruch et al.'s [5], and related foundational works [1–4,6–11]. In addition to the permutation group, graphs are frequently involved in the enumerations, perhaps, with the graph simply providing the skeletal sites as its vertex set and the relevant skeletal permutation group as the graph's automorphism group. See, e.g., [7] or [2,3]. Here, we utilize the graph even further, to invoke a relevant distance function on the sites (and possibly ligands) to modify the simple enumeration problems in a chemically relevant way. But the primacy of these fundamental aspects might be a little further elaborated. With both the skeleton and the ligands represented by graphs, each with their own automorphism group, which in general may involve direct products for each component, and a full automorphism group possibly further involving whole-set-moving permutations which move equivalent sets around themselves. The molecular structures correspond to mappings between skeletal and ligand sets, with constraints then to be implemented by making demands on what happens to the graph edges under such mappings. Disjoint skeletal components under such mappings can become linked through association with a single

multidentate ligand. All this would enable one to deal with coordination complexes which were forefront inorganic research during the first half of the twentieth century. But more generally, the distinction between skeletal and ligand set becomes ambiguous, e.g., with organometallics, which later became the forefront inorganic research. In fact, Pólya used his theory to deal efficiently with the alkanes, where the distinction between skeleton and ligand had the skeleton-ligand nomenclature "submerged" there. In the context of Pólya's framework for our present applications, skeleton and ligand sets are retained, though following Pólya, the ligand set is collapsed into equivalence classes of like ligands, such equivalence classes, then, for a unidentate case being referred to as *colors*, with which the different skeletal sites, then, are to be colored. For a bidentate case, one then has a bicolor to be associated to a pair of (likely adjacency restricted) sites. Thence, we here wish to extend this form of Pólya's theory to retain some information about (molecular) graphical structure underlying the otherwise independent coloring of the different available vertices of the skeletal set.

We associate to any common skeleton S of a family of substitutional isomers a molecular graph $\mathcal{M}(X; E)$ whose set X of vertices (points) correspond to atoms and set E of edges (lines) to neighbor pairs of atoms ($|X| = n$; $|E| = m$); see [7]. To us, of paramount importance are symmetry groups $\text{Aut}\mathcal{M} \cong A$ of automorphisms of $\mathcal{M}$, with members of A represented as permutations acting on the set X of vertices corresponding to the skeleton's sites. Our formalization allows us to consider q-colorings ($q \geq 1$) of vertices of $\mathcal{M}$, in a lieu of really speaking of q sorts of univalent substituents. Thus, we turn to a study of purely combinatorial actions of groups A ($\text{Aut}\mathcal{M}$) on their support sets X. Mathematics can address such problems in an abstract and universal way, as we discuss.

However, before the details of our treatment, we first briefly sketch some background. Here, one of the best books for a reference with a few chapters devoted to enumeration of chemical objects (substitutional isomers etc.) is [7]. Its editor Prof. Alexandru Balaban is himself a famous contributor, who has published over a period of years a large number of related texts which are widely cited in chemistry. But there are numerous other reviews or books focusing on chemical chemical applications [1,8–11].

A simple task is to count up the number of unrestricted substitutional isomers having a skeleton S with a set of sites X (serving also as the vertex set for its graph $\mathcal{M}$), and an automorphism group $A = \text{Aut}\mathcal{M}$, while the number of sorts of ligands is $q \geq 1$. This problem can be solved using the Cauchy-Frobenius lemma (sometimes referred to as Burnside's lemma) and more completely using Pólya's cycle index and associated counting theorem. Aside from [7], purely mathematical literature exists, including: two versions [2,3] of a book by the famous German mathematician Adalbert Kerber; a special book on graph enumerations [4] by celebrated graph theorists Harary and Palmer; and the original classic articles by Pólya [1], De Bruijn [6], Rota and Smith [14]. The mentioned mathematical tools have been expounded and applied also in dozens of more general combinatorics texts and hundreds of papers. The mentioned methodology is most familiar but not unique, and different powerful methods have also appeared over the last 30–40 years, especially ones using double cosets [5] or Burnside's table of marks [2,3].

A second task is to enumerate stereo isomers. The same general tools [1–7, 12, 13, 15–17] are used, working with appropriately selected subgroups of $A = \text{Aut}\mathcal{M}$. Often, the choice for the diastereomers is the same as for the simple substitutional isomers (at least when the skeleton is rigid). The difference between the number of stereomers and the number of diastereomers is the number of enantiomeric pairs.

A third task refines the enumeration to that of isomers with each possible subgroup of symmetry. Here, methods described in [2, 3, 5, 10, 11] are applicable. The final classification of substitutional isomers with respect to their own symmetry groups is performed using the general inclusion-exclusion procedure involving the combinatorial Möbius function [2, 3, 11], perhaps by way of Burnside's "marks" [9, 10]. This entails groups corresponding to each subgroup $H \subseteq A$ in the lattice of subgroups of A. Note, however, that the phrase "each subgroup H" admits, in this case, a more economic algorithm using just certain subgroups, termed "closed", as explicated in [14–17], and later, herein.

Although combinatorics can itself study countable objects without taking into account their physicochemical nature, the chemist should exercise special care of setting combinatorial mathematical character correctly, taking into account relevant physicochemical conditions of each specific problem. Without the last, what is absolutely true from the mathematical point of view may sometimes render an answer to a secondary question. A modest historical instance was the enumeration of 'chemical trees', which interested Cayley, Pólya (see [1]), and other mathematicians (see [2–4, 7]), now for over a century. It was seen that molecules of alkanes can be depicted by their hydrogen-depleted molecular graphs (namely, trees) having only vertex degrees 1, 2, 3, and 4, whence a correct formal enumeration of all chemical trees was successfully formulated. But not all these graphs can be realized in nature as molecules of alkanes, since "steric hindrance" must eventually enforce a taboo upon molecules where different atoms might otherwise theoretically share the same coordinates. In order to bypass this obstacle, nature might only produce much strained molecules with distorted angles between bonds and a severe steric repulsion, so strong as to think that such molecules might not actually be realizable. A new problem thereby arose: How to enumerate molecules of alkanes which do exist? But this question still remains without a complete answer. The overall solution will be possible only after imposing proper constraints on the count, say, by restricting trees to those embeddable on the diamond network, as in [18]. However, we do not here try to solve this problem. Yet another sort of complication entails situations where the relevant symmetry group acts both on site & ligand labels, say in correlated fashion [19–21].

For any real skeleton, there can always be found ligands that are 'too large' to simultaneously occupy adjacent sites. Moreover, this situation may be aggravated by the presence of groups with a strong electrostatic repulsion, or else with mutual reactivity and elimination of the product. As a result, any sort of congestion that forbids the existence of such substitutional isomers makes unrealistic the unrestricted enumeration of general-type colorings of vertices in associated molecular graphs. One may seek to count the restricted colorings of graphs where no two vertices of a selected color are adjacent [12]. One may also increase an allowed minimum distance between a pair of vertices and consider instead a criterion of the exclusion of next-nearest sites to allow

only third-nearest ones *et seq.* such as considered [22,23] whence all colors are so constrained. Such tasks can be addressed using our approach.

Yet further, structural restrictions on substitutional isomers arise. Say, looking for all patterns where attached ligands of a certain type are excluded from certain fixed sites, as might occur because of the presence of certain geometric or topological substructures. An example entailing the introduction of similar refinements upon the usual count of isomers is found in a recent paper [24] by Vukičević and Graovac, who studied optimal configurations of substituents in functionalized fullerenes $C_{60}X_n$ for $n = 2, 4, 6, 8$. Another article [13] studies decarboxylation isomers with restricted positions for de-carboxylations in malonic-acid residues attached to a fullerene molecule C_{60}, where restrictions allow no more than one decarboxylation in each malonic-acid residue. A practically important type of constraint emerges also in case of substitutional isomers containing bidentate ligands, where the two parts ("teeth") of the bidentate ligand often must occupy neighboring sites. Such constraints make attractive novel problems for mathematicians and mathematical chemists.

At this juncture, we turn to a more rigorous exposition, which will, however, be performed in a reader-friendly way, "with a peaceful human voice amidst wild jungles".

2 Preliminaries

This section will be devoted to an exposition of rather rigorous mathematical notions and tools [1–52]. Some other relevant aspects accompanying the topic might also be included in a more extensive discussion, but this is not done herein, where greater focus is sought.

2.1 Setting of the problem using the F-polynomials of graphs

Inasmuch as we use molecular graphs to represent substitutional isomers, this encodes combinatorial graph-theoretic information about their chemical composition (and, possibly, their symmetry and some aspects of their geometry, and/or topology). We seek a census of all significant molecular substructures, which may bear weights for evaluating their individual contribution to the total molecular structure. In graph-theoretical terms, our task is stated as the enumeration of equivalence classes of certain vertex covers of a graph with components drawn from a given collection of its (weighted) subgraphs. The components in these covers, in general, include isolated vertices or edges, or cycles, etc., and yet further take into account restrictions imposed thereon (say, allowed distances between pairs of ligands (or colors), symmetry of a resulting pattern, and whatever else).

Thus, we want first to consider here, a special sort of generating function whose coefficients enumerate symmetry equivalence classes of such vertex covers with respective allowed compositions of subgraphs. We propose the addition of such generating functions to the class of *graph polynomials* in graph theory.

In 1979, the famous mathematician of Trinidad Edward J. Farrell introduced [25] the so-called "family polynomials", or just "F-polynomials" such as encompass many

familiar graph polynomials, including the cycle (circuit), characteristic, matching, permanental, tree, star, path, and clique polynomials. This family is defined in terms of a graph G and a family F of connected and isomorphically distinct graphs. An F-*cover of G* is a spanning subgraph of G, in which every component is isomorphic to a member of F. Let us associate with each member f of F an indeterminate, or weight, w_f, which conventionally then is also the weight of isomorphic copies in G. The *weight of a cover* C, denoted by $w(\mathsf{C})$, is the product of the weights of all its components. Then, the *F-polynomial* is

$$F(G; \mathbf{w}) := \sum w(\mathsf{C}), \qquad (1)$$

where the summation is taken over all the F-covers of G, and where $\mathbf{w}$ is a vector of the indeterminates w_f of $f \in F$.

Note here that the R. H. S. of (1) allows a more general interpretation of the F-polynomial where the $w(C)$ are more general than just $\prod w_f$. Indeed, though not done in [25], this agrees Farrell's opinion (as was stated via correspondence). Generally, (1) may be contemplated for any set of weights that one may attach to the covers C, in it, and even without any relation to the weights w_f. Later, we utilize such a possibility for our goals. Another possibility is to allow the w_f to be from a more general algebra—say, as operators for a "wave operator" to form "cluster expanded" wave-functions, e.g., [26].

Still, as well as in the original examples [25], we shall use throughout this paper a family F of subgraphs f with weights w_f uniquely specified by the number of vertices in f. In particular, this can be applied to every path, star, clique or cycle. Herein, we shall confine ourselves by considering just the cycle case, with the convention that a one-vertex cycle with the weight w_1 is a self-loop or simply an isolated vertex, and a two-vertex cycle with the weight w_2 is an edge (res. a pair of opposite arcs). Then, there follow a triangle, quadrangle, and longer i-cycles with the weights w_3, w_4, and $w_i (i \geq 5)$, consecutively.

As a case in point, choose first Farrell's cycle (circuit) polynomial $Cyc(K_4; \mathbf{w})$ of the complete graph K_4 (the graph of the tetrahedron), viz.:

$$Cyc(K_4; \mathbf{w}) = w_1^4 + 6w_1^2 w_2 + 4w_1 w_3 + 3w_2^2 + 3w_4, \qquad (2)$$

where the five coefficients on the R. H. S. play the following roles: the first, 1 of w_1^4 indicates that there is just 1 spanning K_4 subgraph composed from 4 isolated vertices; the second, 6 of $w_1^2 w_2$ says that there are exactly 6 spanning subgraphs containing two isolated vertices & one edge; the third, 4 of $w_1 w_3$ stands for 4 spanning subgraphs composed from one isolated vertex and one triangle; the fourth, 3 of w_2^2 is for the 3 spanning subgraphs consisting of two disjoint edges; and fifth, 3 of w_4 conveys the occurence of 3 quadrangles, in K_4.

One of the principle goals of Farrell's work, presented by more than a hundred of his (and coauthors') papers (see his site on the Internet), is to study all possible interrelations among different sorts and types of graph polynomials—chiefly based on the F-polynomials. In particular, it was demonstrated that his form of the cycle (circuit) polynomial, whose instance is (2), allows with different substitutions for its variables

$w_1, w_2, \ldots, w_n$ to obtain the characteristic, permanental, and matching polynomials [25,27–33]. But also this yields many other relevant polynomials, such as the Pauling-Wheland overlap function [34,35], with $w_{\text{odd}} = 0$, $w_2 = 2$, and $w_{2n} = 4$, $n \geq 2$. Since we need to consider further the properties of the matching polynomial $M(G; \mathbf{w})$, we note a case in point, using the substitution of 0: $w_i = 0$ for $i \geq 3$ on the R. H. S. of (2), to derive

$$M(K_4; \mathbf{w}) = w_1^4 + 6w_1^2 w_2 + 3w_2^2. \tag{3}$$

This is given in the same n-variable form of its R. H. S. that was originally introduced by Farrell [25,29] for the F-polynomials, and is also the same as the (even earlier) statistical mechanical form with w_1 and w_2 identified as monomer and dimer Boltzmann factors, or activities—e.g., [36]. Aside from defining this matching polynomial as a suitable special case of the cycle polynomial, it can directly be concisely defined as the F-polynomial with $F = \{K_1, K_2\}$. Here, it should be noted that there is another common form $M(G; x)$ of the matching polynomial in one variable x, as defined by the well-known Yugoslav (Serbian) mathematician and chemist Ivan Gutman [30]. In order to obtain the latter, we substitute $w_1 = x$ and $w_2 = 1$ in (3), which results in a signless one-variable form of Gutman's polynomial

$$M(G; x) = x^4 + 6x^2 + 3, \tag{4}$$

which is an equivalent form which can be converted into (3). Such manipulations should enhance our further discussion, when we make some mutual comparisons of the cycle (circuit) polynomial with Pólya's cycle indicator. Now, each individual term in (2) looks like a product $\prod_{i=1}^n w_i^{\sigma_i}$, where σ_i is the number of cycles of length i in a respective C-cover of our graph G. Taking this into account, one can formulate the following elementary but important rule:

Rule 1 *For each individual term $\prod_{i=1}^n w_i^{\sigma_i}$ of the cycle (circuit) polynomial $Cyc(G; \mathbf{w})$ of a graph G on n vertices, $\sum_i^n i\sigma_i = n$ (see [25,27–29]).*

Just this relation can be used for the reverse passage from the R. H. S. of (4) to the R. H. S. of (3), which obviously involves here only w_1- and/or w_2-containing terms out of the entire set of indeterminates $\{w_1, w_2, \ldots, w_n\}$ which may occur in general. Alternatively, in our example, we can employ an individual definition of the matching polynomial with a special notation for the coefficients as is particularly used by Gutman [30]. Namely, the *matching polynomial* of a simple graph G (undirected, unweighted, without self-loops and multiple edges) is taken as

$$M(G; \mathbf{w}) = w_1^n + \mu(G; 1)w_1^{n-2} w_2 + \cdots + \mu(G; h)w_2^h = \sum_{k=0}^h \mu(G; k)w_1^{n-2k} w_2^k$$

$$(\mu(G; 0) := 1), \tag{5}$$

where $\mu(G; k)$ is the number of k-matchings of a graph G, alternatively expressed as the number placements of k nonincident edges in G (with no vertex in common);

and h is the maximum possible number of such placements (in general, $h \leq \lfloor n/2 \rfloor$, so that, often, $\lfloor n/2 \rfloor$ is used instead of h in (5), which admits that $\mu(G; \lfloor n/2 \rfloor)$ may, sometimes, $= 0$; but h is used to identify the last nonzero coefficient $\mu(G; h)$ in (5)).

The coefficients $\mu(G; k)(1 \leq k \leq h)$ are relevant to the problem of enumerations of placements of k bidentate ligands in a common skeleton $\mathcal{S}$ of any admissible substitutional isomers (so long as the connection between the 2 attaching pieces of the bidentate ligand are sufficiently short, as is common). Since our task is to take into account, along with bidentate ligands, unidentate ones also, we want to make yet one refinement of the matching polynomial (say, of the version (5)) using extra auxiliary variables. To this end, we introduce here, besides $\mathbf{w}$, an additional vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ of individual isolated-vertex (res. self-loop) indeterminates where each component x_i is specially associated to the ith vertex of a graph G; it may be considered instead of a common vertex (self-loop) variable w_1 and be also used in a special operational calculus involving partial derivatives of the polynomial $M(G; \mathbf{x}; \mathbf{w})$ with respect to these variables [31–33,37–39] (as below). For instance, we consider the polynomial $M(K_4; \mathbf{x}, \mathbf{w})$, which is a more detailed version of the one in (3), viz.:

$$
\begin{aligned}
M(K_4; \mathbf{x}, \mathbf{w}) = {} & x_1 x_2 x_3 x_4 + x_1 x_2 w_2 + x_1 x_3 w_2 + x_1 x_4 w_2 \\
& + x_2 x_3 w_2 + x_2 x_4 w_2 + x_3 x_4 w_2 + 3 w_2^2,
\end{aligned}
\tag{6}
$$

where individual vertex indeterminates $x_i (1 \leq i \leq 4)$ are associated with the ith vertex of G, in place of a previous common one w_1.

By way of illustration, we want also to show an instance of differential operations with $M(G; \mathbf{x}; \mathbf{w})$; some other cases involving partial derivatives will specially be considered later. First, recall that an *induced subgraph* G^* of a graph G is obtained by deleting a subset of vertices from the latter together with all edges that are incident to them. Let $V(G^*)$ be the vertex set of an induced subgraph $G^* \subset G(|V(G^*)| = n - p < n)$, then (see [31–33])

$$
\frac{\partial^p}{\partial x_{i_1} \partial x_{i_2} \cdots \partial x_{i_p}} M(G; \mathbf{x}, \mathbf{w}) = M(G^*; \mathbf{x}, \mathbf{w}) \quad (i_s \in V(G) \setminus V(G^*); \quad 1 \leq s \leq p),
\tag{7}
$$

where it is understood that $p = 0$ gives the identity in case $G^* = G$. Similarly, more specialized variables x_i can be introduced in the original cycle (circuit) polynomial $Cyc(G; \mathbf{w})$ and any other F-polynomial $F(G; \mathbf{w})$; but in all such cases, the partial derivatives play the same role as in (7). Also, note that left multiplication by an arbitrary constant (weight) w on both sides of (7) conserves the equality. But the main differential manipulations arise in a later subsection. Right now, we continue listing polynomials of potential chemical interest.

From among different graph polynomials which can be used for solving combinatorial problems of chemistry but not explicitly so far related to the F-polynomials, we note two pertinent ones. But first, we need to recollect certain notions. In particular, a *stable* (or *independent*) set (in G) is a set of pairwise nonadjacent vertices of G.
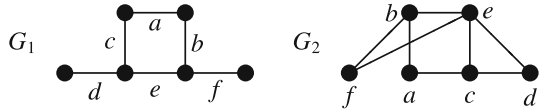
A stable set of the maximum size is referred to as a *maximum stable* set of G, and the *stability*, or *independence, number* $\alpha(G)$ is the maximum cardinality of a stable set in G. Let s_k be the number of stable sets of cardinality k in G.

The polynomial

$$I(G; x) = \sum_{k=0}^{\alpha} s_k x^k = s_0 + s_1 x + s_2 x^2 + \cdots + s_\alpha x^\alpha \qquad (s_0 := 1; \alpha = \alpha(G)) \quad (8)$$

is called the *independence polynomial* of G (Gutman and Harary [40]), or the *independent set polynomial* of G (Hoede and Li [41]). The independence polynomial was defined as a generalization of the *matching generating polynomial* $M(G; x)$ of a graph G [40], which was another version of the matching polynomial, viz.:

$$M(G; x) = x^n M\left(G; \frac{1}{x}\right) = \sum_{k=0}^{h} \mu(G; k) x^k. \quad (9)$$

The main reason for utilizing this relation between the two polynomials was the fact that the matching generating polynomial of a graph G and the independence polynomial of its line graph $L(G)$ are identical. Recall that given a graph G, its *line graph* $L(G)$ is the graph whose vertex set is the edge set of G, and two vertices (of $L(G)$) are adjacent iff (if and only if) they share an end point in G. For instance, the graphs G_1 and G_2 depicted in Fig. 1 satisfy $G_2 = L(G_1)$ and, hence, $I(G_2; x) = 1 + 6x + 7x^2 + x^3 = M(G_1; x)$, where $M(G_1; x)$ is the matching generating polynomial of the graph G_1. In a wider context, to any simple graph G with a family F of connected subgraphs (see the definition of the F-polynomial above), one can associate a derivative graph G_F having the set $F(G)$ of subgraphs isomorphic to the $\mathsf{f} \in F$, as its vertex set wherein two vertices (subgraphs) $\mathsf{f}_1, \mathsf{f}_2 \in F(G)$ are adjacent iff $\mathsf{f}_1 \cap \mathsf{f}_2 \neq \emptyset$. Then, in general, we can write down for a generalized independence polynomial $I(G_F; x)$ of G_F:

$$I(G_F; x) = F(G; 1, 1, \ldots, 1; 1, x, \ldots, x), \quad (10)$$

where $F(G; \cdots)$ is the indicated value of the F-polynomial, of a graph G, associated with a family F; and the substitution of x for variables w_i begins only upon the exhaustion of "simpler" subgraphs in F. This equality (10) indicates a kinship of the independence polynomials to F-polynomials, and concomitantly poses the following question: How should one characterize graphs which are the derivative graphs G_F for given (res. some) families F of connected graphs? The characterization of line graphs (i.e., when F is a family of all edges of G) was proven by Beineke [42,43]. He showed

that there are nine minimal graphs which are not line graphs, such that any graph that is not a line graph has one of these nine graphs as an induced subgraph. That is, a graph is a line graph if and only if no subset of its vertices induces one of these nine graphs. The independence polynomial is also applied to solving different problems of (mathematical) chemistry [44], statistical mechanics [45,46], and, potentially, of many other fields.

In mathematics, a *strict*, or *proper, coloring* of vertices of a graph G using q colors is one where no two vertices of the same color are adjacent. (See the further development of this notion [27,28] by Italian mathematician Mario Gionfriddo, a known expert in generalized colorings, who considers also nonadjacent vertices at fixed distances.) There is a minimum number χ of colors that can be used to obtain such strict colorings, and is called the *chromatic number*. For all bipartite graphs (e.g., of alternant hydrocarbons) $\chi = 2$; so that these are also called bichromatic graphs. It is apparent that a necessary (and sufficient) condition for the existence of a proper coloring of a graph G is $q \geq \chi(G)$. The greater q, the greater is the number of possible n-colorings. The polynomial $Chr(G; x)$ whose coefficients (in x^n) count strict colorings is called the *chromatic polynomial*, introduced in 1912 by the great mathematician George Birkhoff [47] and is, by now, so widely used in graph theory and its applications are so numerous that it might demand a special book to narrate this. Accordingly, $Chr(G; q)$ is equal to the number of strict colorings of a graph G using exactly $q \geq 1$ colors; in particular, $Chr(G; q) = 0$ when $q < \chi$ and $Chr(G; q) > 0$ when $q \geq \chi$. As was already mentioned above, the colors can symbolize different sorts of ligands that should be substituted to a skeleton, so as to avoid the adjacency of two ligands of the same sort. Say, anions and cations in a crystal lattice avoid a close neighborhood of particles possessing like charges. Moreover, notice also that the roots of the chromatic polynomial can also bear some constructional information about a (molecular) graph, say, such as the indication of existence or nonexistence of Hamiltonian paths in it [48].

2.2 A modified Pólya's cycle indicator

Without exaggeration, one may say that the works of Redfield (see Redfield [4]) and Pólya [1] founded the basis modern theory of symmetry-mediated enumeration of objects by the automorphism group (see [2–4,10]). The main mathematical tool that had been known earlier was the Cauchy-Frobenius lemma (often called "Burnside's lemma"). Pólya utilized this fundamental result for the derivation of his celebrated counting theorem and introduced into mathematical practice a special generating function now called Pólya's *cycle index* (or *cycle indicator*) [1]. Although there appeared different powerful methods, say, employing double cosets [5] and Burnside's table of marks (see [2,3]), Pólya's cycle index [1] and its refinements have continued to develop (see [2–4,6,7,10,11] and the two books with translations of [1], nested in the References together with [1]).

Let $A = \mathrm{Aut}X$ be the automorphism (or permutation) group acting on a nonempty finite set X of objects, as above. As was shown by Pólya [1], *A-equivalence classes of objects*, or *A-orbits*, can be enumerated by weight, by means of the special polynomial $C(A; X; s_1, s_2, \ldots, s_n)$ called the *cycle indicator* (or *index*) [1–4,6,15–17]. It may be written down as follows:

$$C(A; X) = C(A; X; s_1, s_2, \ldots, s_n) = \frac{1}{|A|} \sum_{g \in A} \prod_{i \, | \, |A|} s_i^{\varsigma_i(<g>)} , \qquad (11)$$

where $|A|$ is the cardinality of A; s_i's are weight-indeterminates used for convenience of notation; $\varsigma_i(\langle g \rangle)$ 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 $|A|$. Note that here we change the standard notation $\varsigma_i(g)$ to a new, equivalent, notation $\varsigma_i(\langle g \rangle)$ not in vain but because we shall contravene the old tradition to utilize for enumeration purposes just cyclic (1-generator) subgroups and further allow subgroups $\langle g\hat{H} \rangle$ generated by the complete coset $g\hat{H}$ of the normalizer $N_A(\hat{H})$ of $\hat{H}$ in A (see [15–17]). Besides, here we employed not in vain a varsigma version "ς" of the character "σ", previously used in formulation of the Rule 1 for literal terms of the F-polynomials. We choose such a connotation, because all literal terms of cycle indicators also obey our earlier Rule 1. As was already briefly mentioned above, just this similarity in the properties of literal terms of the F-polynomials of graphs and cycle indices makes it possible to extend the general combinatorial results of [15–17] to the case of the generating functions under consideration.

Let $K = \{c_1, c_2, \ldots, c_{|K|}\}$ be a set of weight-indeterminates standing for $|K|$ distinct colors, or simply 'a set of colors'. The following statement is a version of Pólya's counting theorem [1–4,6,15–17], viz.:

Theorem 1 *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*

$$C(A; X; c_1, c_2, \ldots, c_n) = C(A; X; s_1, s_2, \ldots, s_n) \Big|_{s_i = \sum_{t=1}^{|K|} c_t^i \ (i \, | \, |A|)} . \qquad (12)$$

A subgroup $H \subseteq A$ was called *closed* and *periodic* by Rota and Smith [14], or *automorphic* synonymously by us [15–17], 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 $H^g = gHg^{-1} = H'$ is termed an *inner automorphism of H* if $g \in H$, and an *outer automorphism of H* if $H' = H$ while classes are not preserved. Subgroups H and H' actually are distinct but are *conjugate subgroups* in A. Note that if an element $g \notin H$ commutes with H as a whole ($gH = Hg$), then $H' = H$, i.e., the result H^g might still be (equivalent to) an inner automorphism (if classes are preserved).

The notion of subgroup conjugacy permits an important economy in practical combinatorial applications of (symmetry) groups, because every pair of conjugated subgroups always produces essentially the same combinatorial action. In particular, this means that each substitutional isomer is represented by the whole collection of conjugate $g \in G$ for if one conformation c of a substitutional isomer manifests H as a symmetry group, then transforming c by $g \in G$ yields a new conformation of the same isomer now with the symmetry group H^g. Note that this is universally true for

every pair of conjugated subgroups, whether these are closed or not (i.e., for any pair H and H^g; $H, H^g \subseteq A$).

At this stage of our exposition, we are prepared to turn to the solution of some actual tasks of practical use to chemistry, and other fields.

3 Illustrative application: Poly-*t*-butyl derivatives of $B_{12}H_{12}^{2-}$

The dodecahydroborane dianion $B_{12}H_{12}^{2-}$ is an example of a molecular entity having the point symmetry group I_h of cardinality ($|I_h| = 120$). The general interest in diverse hydroborane compounds, we consider the poly-*t*-butyl derivatives of this interesting dianion.

The graph G of the icosahedron, with 12 vertices and 30 edges, plays in our example the role of a skeleton (with sites corresponding to boron atoms) while butyl radicals are the ligands (substituted for hydrogen atoms in the pristine dodecaborane anion). We adopt the numeration of vertices of the icosahedron graph given in Fig. 1 of [53]. Accordingly, we have the following list of edges $e_k = (i, j)(1 \leq k \leq 30; 1 \leq i < j \leq 12)$:

$e_1 = (1, 2), e_2 = (1, 3), e_3 = (1, 4), e_4 = (1, 5), e_5 = (1, 6), e_6 = (2, 3), e_7 = (2, 6),$ $e_8 = (2, 7), e_9 = (2, 11), e_{10} = (3, 4), e_{11} = (3, 7), e_{12} = (3, 8), e_{13} = (4, 5), e_{14} = (4, 8), e_{15} = (4, 9), e_{16} = (5, 6), e_{17} = (5, 9), e_{18} = (5, 10), e_{19} = (6, 10), e_{20} = (6, 11), e_{21} = (7, 8), e_{22} = (7, 11), e_{23} = (7, 12), e_{24} = (8, 9), e_{25} = (8, 12), e_{26} = (9, 10), e_{27} = (9, 12), e_{28} = (10, 11), e_{29} = (10, 12), e_{30} = (11, 12).$

Since *t*-butyl radicals $-C(CH_3)_3$ are sufficiently bulky when substituted at adjacent boron atoms, the problem on placing ligands with exclusive positions is here reduced to that of finding all nonequivalent independent sets of (pairwise nonadjacent) vertices in G. Thus, in particular, information about all (including symmetry equivalent) substitutions of exclusive *t*-butyls to $B_{12}H_{12}^{2-}$ is kept by the coefficients of the ordinary independence polynomial $I(G; x)$. Here, the computation of $I(G; x)$ can be reduced to finding respective edge-disjoint copies of star subgraphs $K_{1,5}$. The edge list $\theta_i = \{k_{i1}, k_{i2}, \ldots, k_{i5}\}(1 \leq i \leq 12; 1 \leq k_{i1} < k_{i2}, < \cdots < k_{i5} \leq 30)$ for each isomorphic copy of $K_{1,5}$ in G as centered at vertex i (consistently with [53]) is: $\theta_1 = \{1, 2, 3, 4, 5\}, \theta_2 = \{1, 6, 7, 8, 9\}, \theta_3 = \{2, 6, 10, 11, 12\}, \theta_4 = \{3, 10, 13, 14, 15\}, \theta_5 = \{4, 13, 16, 17, 18\}, \theta_6 = \{5, 7, 16, 19, 20\}, \theta_7 = \{8, 11, 21, 22, 23\}, \theta_8 = \{12, 14, 21, 24, 25\}, \theta_9 = \{15, 17, 24, 26, 27\}, \theta_{10} = \{18, 19, 26, 28, 29\}, \theta_{11} = \{9, 20, 22, 28, 30\}, \theta_{12} = \{23, 25, 27, 29, 30\}.$

An analytical expression for $I(G, x)$ represented in a differential-operator form is:

$$
I(G; x) = \left\{ \left[\prod_{i=1}^{12} \left(\frac{\partial}{\partial \xi} + x \frac{\partial^5}{\partial y_{i1} \partial y_{i2} \cdots \partial y_{i5}} \right) \right] e^\xi \prod_{j=1}^{30} y_j \right\} \Bigg|_{\xi=0; y_j=1 \ (1 \leq j \leq 30)},
$$

(13)

where ξ, x, and y_j are auxiliary commutative variables; and double indices $i1, i2, \ldots,$ $i5$ correspond to the ordinal numbers of the five edges in θ_i, the ith isomorph of sub-

graph $K_{1,5}$ in G. Algorithmically, the calculation of $I(G; x)$ using (13) includes the stages of successive introduction of new variables y_j now involved in the action of the differential operator $(\cdots)$ in the operator product and (then) of the deletion of those variables y_j which will not be involved in further operations. In a ready form, we obtain

$$I(G; x) = 1 + 12x + 36x^2 + 20x^3, \tag{14}$$

where the coefficient of x^s ($0 \le s \le 3$) is equal to the number of independent sets of s vertices in G (and the maximal such sets contain 3 vertices).

Since $I(G; x)$ itself enumerates all possible independent sets, but not symmetry-equivalent classes thereof, we need a special generalization of Pólya's cycle index to obtain a suitable hybrid of this and the independence polynomial of the icosahedron graph $G\left(\text{of } B_{12}H_{12}^{2-}\right)$. But, first, we calculate the original Pólya's cycle indicator for the permutation representation of point-symmetry group I_h acting on the set $X = V(G)$ of G.

The group I_h has formally 10 classes of conjugated elements but it is worth noting that a pair of classes of elements of order 5 as well as a pair with elements of order 10 are represented, on X, by permutations with equal distributions into cycles (i.e., all elements of order 5 are here combinatorially equivalent, and all elements of order 10 are equivalent). Nonetheless, we give all conjugated classes independently of their mutual correlations, since in general, for other groups, such similarity in actions often does not occur. The elements of symmetry of icosahedron are: the identity (1), rotations about the twofold axis crossing the centers of opposite edges (15), rotations about the threefold axis crossing the centers of opposite facets (20), rotations about the fivefold axis crossing opposite vertices (12 by 72° and 12 by 144°), which all comprise subgroup $I \subset I_h$, and, then, inversion (1), mirror planes crossing the centers of opposite edges (15), mirror rotations of order 6 relevant to the threefold axes (20), mirror rotations of order 10 relevant to both subtypes of fivefold axes (12 + 12), or 120 elements in toto. With the numbering of vertices from [53], representatives of the respective conjugated classes of permutations are:
$g_1 = (1)(2)(3)(4)(5)(6)(7)(8)(9)(10)(11)(12)$; $g_2 = \underline{(1, 2)}(3, 6)(4, 11)(5, 7)(8, 10)$ $(9, 12)$; $g_3 = \underline{(1, 4, 3)}(2, 5, 8)(6, 9, 7)(10, 12, 11)$; $g_4 = (1)(12)\underline{(2, 6, 5, 4, 3)}$ $\underline{(7, 11, 10, 9, 8)}$; $g_5 = (1)(12)(2, 5, 3, 6, 4)(7, 10, 8, 11, 9)$; $g_6 = (1, 12)\underline{(2, 9)}(3, 10)$ $(4, 11)(5, 7)(6, 8)$; $g_7 = (1, 9)\underline{(2, 12)}\underline{(3, 8)}(4)(5)\underline{(6, 10)}(7)(11)$; $g_8 = \underline{(1, 11, 3, 12,}$ $4, 10)$ $(2, 7, 8, 9, 5, 6)$; $g_9 = (1, 12)\underline{(2, 8, 5, 11, 3, 9, 6, 7, 4, 10)}$; $g_{10} = (1, 12)$ $\underline{(2, 11, 6, 10, 5, 9, 4, 8, 3, 7)}$, where underlining indicates that, within a cycle, there are pairs of adjacent vertices (note that such adjacent vertices are also among vertices fixed by the identity but did not delineate this). Following the order of elements above, the cycle index $C(I_h; X)$ is

$$C(I_h; X) = \frac{1}{120}\Big(s_1^{12} + 15s_2^6 + 20s_3^4 + 12s_1^2s_5^2 + 12s_1^2s_5^2 + s_2^6$$
$$+ 15s_1^4s_2^4 + 20s_6^2 + 12s_2s_{10} + 12s_2s_{10}\Big). \tag{15}$$

Also note that $1/60$ times the sum of the first 5 members in parentheses is equal to the cycle index $C(I; x)$ of the subgroup $I \subset I_h$ acting on the same set X. Since we consider a problem involving only two colors (one for hydrogen atoms and one for t-butyls), we may anticipate the generating function(s) in only one variable x for indicating by a respective superscript just the number of t-butyl substituents. Practically, substituting $(1 + x^j)(1 \leq j \leq 10)$ for s_j in (15) gives the ordinary isomer-counting series

$$
\begin{aligned}
C(I_h; X; x) = \frac{1}{120} \Big[& (1+x)^{12} + 15(1+x^2)^6 + 20(1+x^3)^4 + 12(1+x)^2(1+x^5)^2 \\
& + 12(1+x)^2(1+x^5)^2 + (1+x^2)^6 + 15(1+x)^4(1+x^2)^4 \\
& + 20(1+x^6)^2 + 12(1+x^2)(1+x^{10}) + 12(1+x^2)(1+x^{10}) \Big] \\
= & \, 1 + x + 3x^2 + 5x^3 + 10x^4 + 12x^5 + 18x^6 + 12x^7 + 10x^8 \\
& + 5x^9 + 3x^{10} + x^{11} + x^{12}.
\end{aligned}
\tag{16}
$$

Here, none of the powers of x beyond 3 can correspond to possible sizes of independent sets of vertices in G, if it is needed that $\alpha(G) = 3$. Moreover, even the coefficients of lower powers are exaggerated, in counting independent sets.

Now (14) takes into account all independent sets of G (whether equivalent or not); whereas (16) considers all inequivalent subsets, which however are not necessarily independent. One formulation to get at the desired coefficients is: Substitute for all generating functions summed in square brackets in (16) proper expressions which exactly exclude any adjacency of vertices which are inside one and the same orbit (cycle) or are in different orbits, generated on X, by respective representative (cyclic) subgroups $< g_j >\subset I_h (1 \leq j \leq 10)$. In particular, we have to substitute the R. H. S. of (14) in (16), which is the independence polynomial of G, for $(1+x)^{12}$, and substitute 1 for $(1+x^6)^2$ in (16), because the cyclic group $\langle g_8 \rangle$ reproduces the cycle distribution of its generator $g_8 = \underline{(1, 11, 3, 12, 4, 10)}(2, 7, 8, 9, 5, 6)$ into two orbits containing pairs of adjacent vertices (say, vertices 1 & 3 in one orbit and 2 & 6 in the other), and rejecting both of these orbits (comprising all sites of a skeleton) results in the case of unsubstituted dianion $B_{12}H_{12}^{2-}$. Here, we propose to the reader an exercise: derive all substitutive polynomials using the list of cycle distributions induced by all 10 generators g_j, which preceded (15). The solution is: a hybrid independence-cycle-index polynomial:

$$
\begin{aligned}
IC(I_h; X; x) = \frac{1}{120} \Big[& (1 + 12x + 36x^2 + 20x^3) + 15(1 + 4x^2) + 20(1 + 2x^3) \\
& + 12(1 + 2x + x^2) + 12(1 + 2x + x^2) + (1 + 6x^2) \\
& + 15(1 + 4x + 6x^2 + 4x^3) + 20(1) + 12(1 + x^2) + 12(1 + x^2) \Big] \\
= & \, 1 + x + 2x^2 + x^3.
\end{aligned}
\tag{17}
$$

In the last part of (17), 1 corresponds to an unsubstituted dianion $B_{12}H_{12}^{2-}$ with the full I_h symmetry, x to a C_{5d}-group monosubstituted isomer, one x^2 is assigned to a

(*meta*) disubstituted isomer with symmetry group C_{2v}, the other x^2 to a (*para*) isomer with the group D_{5d}, and the only trisubstituted isomer, indicated by x^3, possesses the symmetry group D_{3d}. The other 17 subgroups of I_h (see [54]) are not represented by *t*-butyl derivatives of $B_{12}H_{12}^{2-}$, which is a consequence of restrictive positions of ligands in a skeleton, considered in our problem.

4 Conclusion

Herein, we have demonstrated the principal possibility to perform this and similar tasks, though weak on a practicable calculational algorithm. Therefore, we consider in a parallel paper the overall analytical approach to solving such problems and its realization using symbolic algebraic calculations with program packages such as Maple.

Owing to certain common properties of all graph polynomials mentioned above, one may make the next step for a general treatment of them. In particular, in our next paper, we specially regard possible symmetry restrictions that may be imposed on the covers **C**, in different tasks.

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