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Graph edge colorings and their chemical applications

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A general method is outlined to enumerate the edge-colorings of graphs under group action. The symmetry group of the graph acting on the vertices induces permutation of the edges. The edge-colorings are enumerated using the edge-permutation group. A number of chemical applications especially to multiple quantum NMR spectroscopy, statistical mechanics, enumeration of unsaturated isomers, etc. are considered.

Key words: Edge group — Edge colorings — NMR — Graph theory — Configuration integral

1. Introduction

There have been a large number of publications in recent years [1-27] which have dealt with applications of combinatorial and graph theoretical techniques to many areas of chemistry such as quantum chemistry, spectroscopy, statistical mechanics, chemical kinetics, drug design and quantum pharmacology. A recent review by the present author [1] summarizes the applications of combinatorics and graph theory especially to quantum chemistry, spectroscopy and stereochemistry.

A graph is simply a diagram of vertices connected by edges which may represent a molecule, hamiltonian operator, statistical mechanical cluster, reaction networks in chemical kinetics, NMR interaction diagrams, etc. The vertex colorings of graphs, alternatively, enumeration of substituted isomers have been studied quite extensively in the chemical literature by many authors [1-5, 13, 14, 28-30]. If various colors represent different types of substituents, then the unique vertex colorings are the various poly-substituted isomers. The edge-colorings of a graph can be defined as the non-equivalent ways one could color the edges of a graph

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such that one coloring is not transformable into another coloring by the edge group acting on the graph. The formulation of edge-colorings of graphs and their chemical applications have not been studied at all by the chemical community. The reason is apparent, namely, the applications are somewhat hidden. There are, however, a wealth of information of chemical and spectroscopic relevance that could be derived from such developments as we demonstrate here.

The edge-colorings of graphs are shown to be useful in multiple quantum NMR from which one could obtain various types of dipolar couplings present in a molecule. The question then is in how many different ways could one assemble these dipolar couplings. Each such way corresponds to a possible structure of the unknown compound. The edge-colorings of graphs are shown to enumerate unique dipolar interactions among a given set of nuclei thereby providing a technique for structure elucidation from NMR.

The edge-colorings of graphs are also shown to have applications in the enumeration of unsaturated isomers of a class of organic compounds. They would also have applications in statistical mechanics in enumerating the number of statistical mechanical diagrams contributing to the configuration integral. Finally, the edge-colorings of graphs could enable classification of Kekulé structures into equivalence classes of structures such that all structures in a class have the same resonance energy. Section 2 describes preliminaries and formalism of the edge group. Section 3 outlines the basic method to enumerate the edge-colorings. Section 4 describes applications.

2. Edge groups

Let $S_v = \{v_1, v_2 \cdots v_n\}$ be the set of vertices of a graph G and let $S_e = \{e_{12} \cdots e_{kl}\}$ be the edges of the graph, where e_{ij} is an edge between the vertices i and j. For example, Fig. 1 shows the complete graph containing four vertices. The set S_v for this graph is $\{v_1, v_2, v_3, v_4\}$ while the set S_e for this graph is $\{e_{12}, e_{13}, e_{14}, e_{23}, e_{24}, e_{34}\}$. The adjacency matrix of a graph is defined as

$$A_{ij} = \begin{cases} 1 & \text{if } i \neq j \text{ and the vertices } i \text{ and } j \text{ are connected} \\ 0 & \text{if } i = j. \end{cases} \tag{1}$$

Note that the order of the adjacency matrix is $n \times n$ if n is the number of vertices. The automorphism group of a graph is defined as the set of permutations of the vertices of the graph which leave the connectivity of the graph invariant. Alternatively, if P is a $n \times n$ permutation matrix which corresponds to a permutation of the vertices of the graph then P belongs to the automorphism group if

$$P^{-1}AP = A. \tag{2}$$

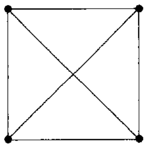


Fig. 1. The complete graph on four vertices (K_4)

It can be easily verified that all such permutations which leave A invariant form a group called the automorphism group of a graph.

We now define another group induced by the automorphism group which is called the edge group. The edge group has been used earlier [30] in enumerating edge colorings of graphs. The automorphism group G_v of a graph permutes the set of vertices, S_v, of a graph. This in turn induces permutation of the edges as follows. Suppose the vertex permutation in G_v is denoted by

$$\begin{pmatrix} 1 & 2 & \cdots & n \\ P_1 & P_2 & \cdots & P_n \end{pmatrix} \tag{3}$$

where the second row represents the permuted vertices, $P_1, P_2 \cdots P_n$ being a permutation of the integers $1 \cdots n$. An edge e_{ij} connecting the vertices i and j will become $e_{p_ip_j}$ under this permutation. The result of the vertex permutation is then the following edge permutation of length p (where p is the number of edges), shown below.

$$\begin{pmatrix} e_{12} & e_{13} & \cdots & e_{kl} \\ e_{p_1p_2} & e_{p_1p_3} & \cdots & e_{p_kp_l} \end{pmatrix}. \tag{4}$$

It can be easily shown that the edge permutations form a group. The order of the edge group is the same as the order of the vertex automorphism group since the two groups are isomorphic except for the K_2 graph for which the edge group is the identity group while the vertex group is S_2. If we denote a group of $n!$ permutations acting on n objects by S_n, then the automorphism group of a graph is a subgroup of S_n, where n is the number of vertices. The edge group, however, would be a subgroup of S_p where p is the total number of edges of the graph.

Let us illustrate the concept of edge group with the example shown in Fig. 1. For Fig. 1, the complete graph on four vertices, K_4, the automorphism group acting on vertices can be easily shown to be the group of 4! permutations. Consider for example the vertex permutation (1)(234). The edge permutation induced by this vertex permutation is shown below

$$\begin{pmatrix} e_{12} & e_{13} & e_{14} & e_{23} & e_{24} & e_{34} \\ e_{13} & e_{14} & e_{12} & e_{34} & e_{23} & e_{24} \end{pmatrix}. \tag{5}$$

Note that in forming the above permutation we use the fact that the edge e_{ij} is the same as e_{ji} for a non-directed graph. The above permutation is isomorphic with a permutation of six objects shown below.

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 2 & 3 & 1 & 6 & 4 & 5 \end{pmatrix}. \tag{6}$$

In cycle notation, the above permutation is denoted by (123)(465) which is a member of the group S_6. The edge group for K_4 then would consist of 4! permutations but is a subgroup of S_6. It can be shown that every vertex permutation in the automorphism group generates a unique edge permutation and thus the number of elements in the edge group would be identical to that of the vertex automorphism group.

3. Edge colorings and their enumeration

The edge-colorings of a graph are defined as the non-equivalent ways of coloring the edges of a graph with a given set of colors. For example, if we had four white colors and two black colors, the graph in Fig. 1 can be colored in two non-equivalent ways shown in Fig. 2, where the black color is denoted by a shaded edge. The problem of edge colorings can be formulated as follows.

Let n_1 be the number of colors of type 1 (black), n_2 be the number of colors of the type 2 (red), n_3 be the number of colors of the type 3 (blue), etc. An edge coloring is defined formally as a mapping f from the set of edges D into the set of colors R defined below.

$$f: D \rightarrow R. \tag{7}$$

For example, one of the two colorings shown in Fig. 2 corresponds to the map shown below.

$$\begin{aligned} f_1: 1 &\rightarrow w \\ 2 &\rightarrow w \\ 3 &\rightarrow w \\ 4 &\rightarrow w \\ 5 &\rightarrow b \\ 6 &\rightarrow b, \end{aligned} \tag{15}$$

where w stands for the white color and b stands for the black color. Let F be the set of all such possible maps. It can be easily seen that there are $|R|^{|D|}$ such maps in F. Two functions f_1 and f_2 are equivalent if there is a permutation g in the edge group G such that

$$f_1(d) = f_2(gd) \quad \text{for all } d \in D. \tag{9}$$

The above relation can be easily checked to be an equivalence relation. Two functions are equivalent if the corresponding colorings are transformable into each other by a member of the edge group. Thus, the above relation divides the set F of all functions into equivalence classes. A member from each equivalence class then corresponds to a unique edge-coloring. The number of non-equivalent edge-colorings is precisely the number of equivalence classes.

The total number of equivalence classes and the number of non-equivalent edge-colorings for a given set of colors can be generated using Pólya's theorem

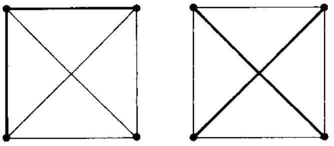


Fig. 2. Two non-equivalent ways of coloring the edges of K_4 with four colors of one type (*white*) and two colors of another type (*black*)

[28-30]. The general formulation and application of Pólya's theorem to a number of chemical problems was reviewed by the present author [1].

Let g be a member of the edge group G of the given graph. Suppose g generates b_1 cycles of length 1, b_2 cycles of length $2 \cdots b_k$ cycles of length $k \cdots$ upon application of g on the edges of the given graph. Then $x_1^{b_1} x_2^{b_2} \cdots x_k^{b_k} \cdots$ is said to be a cycle representation of the edge permutation g. The cycle index of the edge group G is then defined as

$$P_G = \frac{1}{|G|} \sum_{g \in G} x_1^{b_1} x_2^{b_2} \cdots x_k^{b_k} \cdots \tag{10}$$

To illustrate, the cycle representation of the edge permutation (123)(465) generated by the vertex permutation (1)(234) of the K_4 graph (Fig. 1) is x_3^2 (2 cycles of length 3). The cycle index of the edge group of the K_4 graph is given by

$$P_G = \tfrac{1}{24}[x_1^6 + 9x_1^2 x_2^2 + 8x_3^2 + 6x_2 x_4]. \tag{11}$$

Pólya [28] showed that a generating function for the equivalence classes, which for edge-colorings we call the edge-color-inventory (ECI), can be obtained as follows. Let w_1 be the weight assigned to the color of type 1. Let w_2 be assigned to color of the type 2, etc. Then the weight of a map $f: D \to R$ is defined as the product of the weights of the images. Symbolically,

$$W(f) = \prod_{d \in D} w(f(d)). \tag{12}$$

To illustrate the weight of an edge-coloring which contains b_1 colors of the type 1, b_2 colors of the type 2, etc. is given by

$$W(f) = w_1^{b_1} w_2^{b_2} \cdots w_k^{b_k} \cdots \tag{13}$$

The edge-color-inventory (ECI) for the given graph is then obtained by Pólya's theorem as

$$\mathrm{ECI} = P_G\left(x_k \to \sum_{r \in R} (w(r))^k \right). \tag{14}$$

Let us illustrate this procedure with the example of K_4 (Fig. 1) that we have been considering up to now. Let the set R contain just two colors, namely, white and black. Let the weight of the white color be w and the corresponding weight for the balck color be b. Then the ECI is given by

$$\mathrm{ECI} = \tfrac{1}{24}[(w+b)^6 + 9(w+b)^2(w^2+b^2)^2 + 8(w^3+b^3)^2 + 6(w^2+b^2)(w^4+b^4)]. \tag{15}$$

The expression (15) upon simplification leads to expression (16).

$$\mathrm{ECI} = w^6 + w^5 b + 2w^4 b^2 + 3w^3 b^3 + 2w^2 b^4 + wb^5 + b^6. \tag{16}$$

The coefficient of $w^{n_1} b^{n_2}$ in ECI gives the number of non-equivalent ways of coloring K_4 with n_1 white and n_2 black colors. Thus, there is one way of coloring K_4 with six white colors, one way of coloring with five white and one black colors, two ways of coloring with four white and two black colors (shown in Fig.

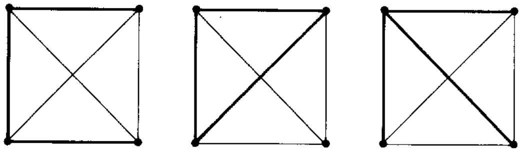


Fig. 3. The three edge colorings of K_4 with three colors of one kind and three colors of another kind

2), three ways of coloring with three white and three black colors, etc. The three ways which correspond to the w^3b^3 term are shown in Fig. 3 since it is not obvious as to what these are. Note that the three shaded edges together constitute the possible unique subgraphs on four vertices which contain three edges.

The above procedure is quite general and powerful in that it can be extended to many colors. Consider for example, three types of colors say green (g), blue (b) and red (r). The generating function for the edge-color-inventory for three types of colors is obtained by replacing every x_k by $g^k+b^k+r^k$ in the cycle index of the edge group. The resulting expression (17) for three types of colors is shown below.

$$\tfrac{1}{24}[(g+b+r)^6+9(g+b+r)^2(g^2+b^2+r^2)^2+8(g^3+b^3+r^3)^2 \\ +6(g^2+b^2+r^2)(g^4+b^4+r^4)]. \qquad (17)$$

The expression (17) upon simplification results in (18)

$$g^6+g^5b+2g^4b^2+3g^3b^3+2g^2b^4+gb^5+b^6+g^5r+2g^4br+4g^3b^2r+4g^2b^3r \\ +2gb^4r+b^5r+2g^4r^2+4g^3br^2+6g^2b^2r^2+4gb^3r^2+2b^4r^2+3g^3r^3 \\ +4g^2br^3+4gb^2r^3+3b^3r^3+2g^2r^4+2gbr^4+2b^2r^4+gr^5+br^5+r^6. \qquad (18)$$

For example, there are six non-equivalent ways of coloring the K_4 graph with two green, two blue and two red colors.

Before we proceed with applications, we give one more example. Consider the complete graph containing five vertices which is denoted as K_5. For this graph, the ECI for two colors is given by (19)

$$w^{10}+w^9b+2w^8b^2+4w^7b^3+6w^6b^4+6w^5b^5+6w^4b^6+4w^3b^7+2w^2b^8 \\ +wb^9+b^{10}. \qquad (19)$$

4. Applications

4.1. *NMR and multiple quantum NMR*

We start with the definition of an ordinary NMR spin hamiltonian. This is defined as

$$H_{\mathrm{NMR}}=\sum_i \nu_i I_{zi}+\sum_{i<j}\sum J_{ij}\mathbf{I}_i\cdot\mathbf{I}_j \qquad (20)$$

where ν_i is the chemical shift of the ith nucleus, J_{ij} is the isotropic spin-spin coupling constant between the nuclei i and j, I_{zi} is the z-component of the nuclear spin vector; $\mathbf{I}_i \cdot \mathbf{I}_j$ is the scalar product of the spin operators $\mathbf{I}_i$ and $\mathbf{I}_j$. The present author [17] defined the NMR graph of the associated hamiltonian as the diagram of nuclei with the edges representing the J-coupling constants. To illustrate, the NMR graph of the ethane molecule is shown in Fig. 4. Note that in Fig. 4, the edges represent the proton-proton couplings while the vertices are the protons. Carbon nuclei are not shown since we consider ^{12}C-ethane. In Fig. 4, the coupling weight τ corresponds to the H-H coupling of the protons on the same carbon while τ' corresponds to the H-H coupling of two protons on two different carbon atoms.

The NMR graph shown in Fig. 4 corresponds to an edge-coloring of the K_6 graph, namely, a way of coloring the edges of K_6 with six colors of one kind and nine colors of another kind. Thus, there is one-to-one correspondence between a NMR graph and the edge coloring of a complete graph. There are 21 ways of coloring the edges of the K_6 graph with six colors of one kind and nine colors of another kind. The NMR graph of ethane corresponds to one of 21 edge-colorings of K_6.

The question of how many different NMR graphs are possible for a given set of nuclei and coupling constants is an important and fundamental one since it could provide solutions to structure elucidation from NMR. That is, given the distribution of coupling constants if one can construct the possible NMR graphs then one could arrive at possible structures from the NMR graphs.

Pines and coworkers [31, 32] have been considering multiple quantum NMR spectroscopy in liquid crystals as a tool for molecular structure elucidation. The normal NMR spectrum is a 1-quantum spectrum (Zeeman-allowed transitions $\Delta M_F = \pm 1$) and is quite complex for a compound containing many nuclei. For a molecule containing N-protons, the $(N-2)$-quantum spectrum is considerably simpler and yet contains important information on different types of dipolar coupling constants. The NMR hamiltonian for dipolar couplings is similar to the one defined earlier except that the isotropic J-coupling should be replaced by a combination of non-isotropic (oriented) dipolar couplings. The dipolar couplings (D_{ij}) are more useful since they provide direct information on structures. The

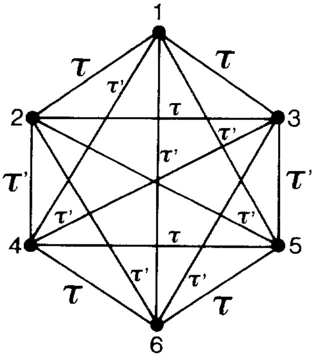


Fig. 4. The NMR graph of ethane

multiple quantum transitions of order greater than eight are difficult to obtain. Thus, Gochin and Pines [32] have devised an ingenious way of deutrating the compound under consideration thereby eliminating many dipolar couplings and reducing the order of the transition.

The random deuteration of protons would lead to isomers containing fewer protons reducing the $(N-2)$ value for the multiple quantum NMR. Random deutration leads to a large number of isomers, in general. The problem then is the following. Given the number and types of dipolar couplings and the number of proton nuclei could one enumerate the possible NMR graphs so that one could assign the observed spectrum to the appropriate isomers?

The problem of constructing the possible NMR graphs given the dipolar couplings can be formulated as follows. Let R be the set of dipolar couplings containing n_1 couplings of the type 1 (D), n_2 couplings of the type 2 (D'), n_3 couplings of the type 3 (D''), etc. Let n be the number of protons. Then it can be seen from our earlier results and discussions in Sect. 3 that the number of different types of NMR graphs is precisely the number of edge-colorings of K_n with the above distribution of colors, namely, n_1 colors of the type 1, n_2 colors of the type 2, etc. This is precisely the coefficient of $w_1^{n_1} w_2^{n_2} \cdots$ in the ECI (edge-color inventory) (see the previous section). For the K_6 graph, we show below the ECI for two types of colors (white and black)

$$\begin{aligned} &w^{15}+w^{14}b+2w^{13}b^2+5w^{12}b^3+9w^{11}b^4+15w^{10}b^5+21w^9b^6+24w^8b^7 \\ &\quad+24w^7b^8+21w^6b^9+15w^5b^{10}+9w^4b^{11}+5w^3b^{12}+2w^2b^{13}+wb^{14}+b^{15}. \end{aligned} \tag{21}$$

Thus, there are two NMR graphs containing six nuclei with 13 couplings of one kind, two couplings of the other kind (coefficient of $w^{13}b^2$), five graphs with 12 couplings of one kind, three of the other kind (coefficient of $w^{12}b^3$), etc.

4.2. Enumeration of positional isomers of unsaturated organic compounds

A standard problem in organic chemistry is the enumeration of structural isomers (positional isomers) of unsaturated compounds. For example, Fig. 5 shows the two positional isomers of butadiene (1, 2 and 1, 3). The question of enumerating positional isomers of unsaturated compounds reduces to an edge-coloring problem. In how many ways could one color a molecular graph with n_1 colors of the type 1 (single bonds), n_2 colors of the type 2 (double bonds), n_3 colors of the type 3 (triple bonds), etc. such that (i) one coloring is not transformable into another under the action on the automorphism group of the molecular graph and (ii) the tetravalency of the carbon atom is satisfied? The answer to this question is a particular case of the formalism outlined in Sect. 3 for unbranched compounds containing no fused or spiro rings.

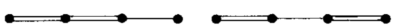


Fig. 5. The two position isomers of butadiene

Consider a linear chain containing six atoms (L_6). For this graph the cycle index of the edge group is given by

$$P_G = \tfrac{1}{2}[x_1^5 + x_1 x_2^2]. \tag{22}$$

The ECI with two colors would enumerate all possible structures containing single and double bonds. If one assigns a symbol s for single bonds and d for double bonds, the ECI is given by

$$\begin{aligned} \mathrm{ECI} &= \tfrac{1}{2}[(s+d)^5 + (s+d)(s^2+d^2)^2] \\ &= s^5 + 3s^4d + 6s^3d^2 + 6s^2d^3 + 3sd^4 + d^5. \end{aligned} \tag{23}$$

Thus, there are three hexenes, six hexadienes, six hexatrienes, etc. Thus the enumeration of edge-colorings of graphs has important applications to structure elucidation.

The presence of branches or fused or spiro rings in the structure presents a problem in that some of the structures enumerated by an ordinary ECI would, in fact, violate the tetravalency of the carbon atom. In this case the edge group should be applied to a restricted set of functions representing the colorings which do not violate the carbon tetravalency. This can be accomplished using the principle of inclusion and exclusion as shown by the present author [4, 34] in an earlier publication on the enumeration of polysubstituted alcohols. However, in using such methods, one loses the analytical simplicity present in the previous example and there are no closed analytical expressions, in general.

4.3. Applications to statistical mechanics

The classical formulation of the canonical partition functions involves a classical configuration integral denoted by Q_N [33], where N is the number of particles. The $3N$-dimentional integral Q_N can be written as

$$Q_N = \int \cdots \int e^{-\beta U}\, d\tau_1 \cdots d\tau_N, \tag{24}$$

where U is the total potential term which can be expressed as a sum of pairwise interaction terms as follows

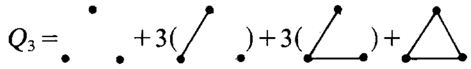
$$U = \sum_{i<j}\sum u(r_{ij}). \tag{25}$$

The configuration integral Q_N can be written in terms of the Mayer function f defined below as,

$$f_{ij} = e^{-\beta u(r_{ij})-1} \tag{26}$$

$$Q_N = \int \cdots \int d\tau_1 \cdots d\tau_N \{1 + \sum f_{ij} + \sum f_{ij} f_{kl} + \cdots\}. \tag{27}$$

A graph theoretical expansion of Q_N can be obtained by representing each of the above integrals by a labelled graph containing N points such that if a factor f_{ij} is present in the integral then the vertices labelled i and j are connected. Such a graph can be called a statistical interaction diagram. The contributions of two integrals to Q_N are the same if the topological structures of the associated graphs are the same. Thus, the number of inequivalent ways of labelling an unlabelled graph and the number of "different" graphs on N points can yield an expansion for Q_N. To illustrate the expansion for Q_3 is shown below:



(28)

The enumeration of "different" graphs on a set of N points can be formulated in terms of edge colorings of a complete graph K_N as follows. If one assigns a weight w if there is an edge and a weight 1 if there is no edge, then the ECI enumerates the number of different graphs on N vertices. For example, the ECI for K_4 and K_6 are given by (29) and (30), respectively.

$$\mathrm{ECI}(K_4) = 1 + w + 2w^2 + 3w^3 + 2w^4 + w^5 + w^6 \tag{29}$$

$$\begin{aligned}\mathrm{ECI}(K_6) = {} & 1 + w + 2w^2 + 5w^3 + 9w^4 + 15w^5 + 21w^6 + 24w^7 + 24w^8 \\ & + 21w^9 + 15w^{10} + 9w^{11} + 5w^{12} + 2w^{13} + w^{14} + w^{15}.\end{aligned} \tag{30}$$

Thus, there is one graph which contains one edge and four vertices (coefficient of w in (29)), two graphs containing two edges (coefficient of w^2), three graphs containing three edges (coefficient of w^3), etc. In general, the coefficients of w^k in expressions (29) and (30) enumerate number of different graphs containing k edges and N vertices for $N=4$ and 6, respectively. All graphs containing four vertices are also enumerated in [30] and are shown in Fig. 6. Once all graphs containing N vertices have been enumerated, the next step would be to find the "weighting factor" for that graph which is simply the number of different ways to label the graph. This number is given by

$$\Omega = \frac{N!}{|G|} \tag{31}$$

where $|G|$ is the number of elements in the vertex automorphism group of the graph. To illustrate, the weight factor for the fourth graph in Fig. 6 is three since the automorphism group of this graph is the wreath product $S_2[S_2]$ whose order

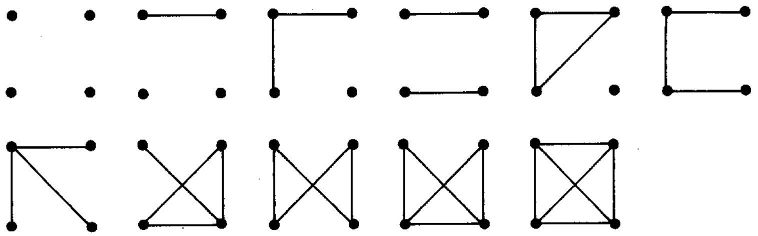
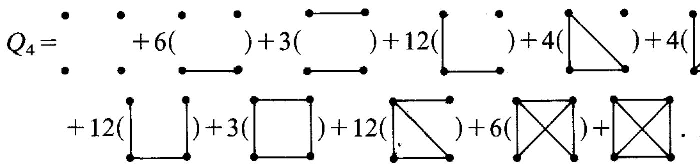


Fig. 6. The eleven non-equivalent graphs containing four vertices. These enumerated by expressions (28)

is 2.2^2. Thus Ω is $4!/8=3$. The final graph theoretical expansion for Q_4 is thus given by (32) which agrees with the result obtained in [33]



(32)

It should be pointed out that further simplification in the final evaluation of the canonical partition function and the virial coefficients is achieved if one enumerates a subset of all the graphs on N points called the Mayer graphs. Mayer graphs or irreducible cluster graphs (irreducible cluster integrals) are connected graphs on N vertices with no cut vertex or an articulation point. A cut vertex is a vertex in a graph which leaves the graph disconnected if it is removed from the graph. The last three graphs in Fig. 4 are the only three Mayer cluster graphs on four vertices.

5. Conclusion

In this investigation, we formulated a group called the edge group of a graph. The enumeration of the edge colorings of a graph was outlined. It was shown that edge colorings of graphs have several important applications in ordinary NMR, multiple quantum NMR, enumeration of positional isomers of unsaturated compounds and the enumeration of irreducible clusters in statistical mechanics.

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