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STATISTICAL PROPERTIES OF FINITE POINT GROUPS OF SYMMETRY

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Abstract

The mean entropy of the distribution of elements of finite point groups of symmetry into classes, irreducible representations and multiplication table is studied and its properties formulated in a number of theorems. It is shown that the mean entropy is the same in the isomorphic groups, and, in the case of the direct product of two groups, it is an additive quantity, equal to the sum of the mean entropies of the two groups. A semiadditivity was also found for the group-subgroup relation.

1. Introduction

The group theory is of great importance for chemistry[1-6]. Contrary to the classical quantitative mathematical methods it describes first of all the different quality of the chemical systems and represents an essential new stage in the mathematisation of chemistry. The symmetry of atoms, molecules, and crystals, reflected in the corresponding groups of symmetry determines to a grꞏat extent their properties and behaviour, and plays an important role in the quantum mechanical description of these systems.

Information Theory[7-11] also reveals new properties of the material systems. Any system having a determined structure carries in itself a corresponding amount of structural information. The interactions which change a certain structure, change its information content as well. In this regard it becomes more and more evident that systems and processes have also an information side, independent of their concrete material essence. Thus, the energetic and the substantial descriptions turn out to be insufficient.

On this basis, any attempts to combine Group Theory and Information Theory, as well as attempts at statistical analysis of the symmetry of various systems will be of interest. Only a small number of such works treating the automorphic groups of molecular graphs[12-14] and the point groups of symmetry[15] have been reported up to now. The information content of molecules is defined in them, denoted as topological information and information for symmetry, respectively. The basic approach in these works is the partitioning of the set of atoms in the molecule into subsets of equivalent atoms. Those atoms are considered equivalent which interchange their places when the operations of the group, to which the molecule belongs, are carried out.

A different approach is possible in principle, i.e., for the statistical properties of the groups themselves to be analyzed and for it to be seen how these properties are reflected in the concrete systems, belonging to a certain group. Any group has an inner structure characterized by a definite amount of entropy. For example, the group may be considered as a definite structure composed of classes of elements, of irreducible representations, of subgroups, etc. In addition any irreducible representation can be considered as a definite structure of characters, etc. In the present work the main results of information theoretic investigations of point groups of symmetry are presented, in which statistical characteristics of the groups are defined, and their properties and changes upon some operations on the groups are studied.

2. Information Theoretic Approach to the Analysis of the Finite Point Groups

In 1948 C.Shannon suggested his formula

$$H(P) = -\sum_{i=1}^{k} p_i . \log_2 p_i \qquad (1)$$

for the entropy of the probability distribution $P = (p_1, p_2, \ldots, p_k)$ of a random variable X, having k different values $(x_1, x_2, \ldots x_k)$.

The equation of Shannon can also be used for characterizing different structures. A finite probability scheme can be constructed for a structure having N elements distributed into k different substructures :

$$\begin{pmatrix} N_1, & N_2, \ldots, & N_k \\ p_1, & p_2, \ldots, & p_k \end{pmatrix}$$

where $\sum N_i = N$, and $p_i = N_i/N$ is a probability of a randomly chosen element to be in the i-th group. The entropy of the probability distribution, determined according to eqn.(1), will be an important statistical characteristic of the structure under consideration*.

H(P) has a maximum when the probability p_i of a certain element being in each of the k-substructures is the same:

$$H(P) = \log_2 k = \max \quad (k = \text{const}) \qquad (2)$$

Since in such a case the events occur with an equal probability, their occurence provides no information. The function reaches its absolute maximum when the number of groups k is equal to the number of structural elements N, since the uncertainty increases if the number of events does so. Conversly, H(P) = 0 when all the elements belong to one group only. In that case the probability of a randomly chosen element being in this group is $p_i = 1$, and the maximum information on this event is available.

* Taking as a measure of structural information its entropy, Shannon's function is often called "information content"[12,13], or "structural information content"[14], or "mean information content" ([15] and other publications of the authors of the present paper) of the structures. Additional justification of this terminology can be found in [16,17] et al.

In this paper any finite point group of order h is considered as a set composed of h elements. Different decompositions of this set into k-subsets, having $N_1, N_2, \ldots, N_k$ elements respectively, are taken into account. Then, the ratio $N_i/h = p_i$ defines the probability p_i of an arbitrary chosen element of the group being in the i-th subset. Making use of Shannon's equation, the entropy of probability distribution in the diverse group decompositions is specified and its properties studied.

Symmetry elements which can be derived from one another by some transformation of the coordinates, consisting of symmetry elements of the same system, form a class. Dealing with the decomposition of the elements of a certain group into k-classes, each one of N_i elements, the mean entropy of probability distribution can be determined, in bits per element, by eqn.(1). Denoting this statistical characteristic of the group by H_G^{Cl} one obtains:

$$H_G^{Cl} = - \sum_{i=1}^{k} N_i/h . \log_2 N_i/h \qquad (3)$$

Another decomposition of h into subsets can be carried out on the basis of the important theorem of the group theory, according to which the order of the group is a sum of the squares of the dimensions of all of its irreducible representations (IR) :

$$h = l_1^2 + l_2^2 + \ldots + l_k^2 \qquad (4)$$

Dealing with the h-dimensional space of the group as composed of k-subspaces, each of them having a dimension l_i^2, a mean entropy of the probability distribution over the irreducible representations of the group H_G^{IR} can be defined. In this case p_i of eqn.(1) will be the probability of an arbitrarily chosen irreducible representation having a dimension l_i :

$$H_G^{IR} = - \sum_{i=1}^{k} l_i^2/h . \log_2 l_i^2/h \qquad (5)$$

The multiplication table of the group is a square matrix composed of h x h symmetry elements. Each symmetry element appears once in every row or column of the table. The set of h^2 elements can be partitioned into h subsets each of which having h identical elements. Specifying the probability of a randomly chosen symmetry element being in the i-th group of identical elements; $p_i = h/h^2 = 1/h$, the mean entropy of matrix elements distribution in the multiplication table of the group can be defined in bits per element :

$$H_G^{MT} = \log_2 h \qquad (6)$$

Another entropy measure, $H_G^{MT'}$, dealing with the multiplication table can be introduced as a structure composed of h rows (or columns). Since there are no two identical rows (or columns) in the table, the set of h elements is decomposed to h subsets of one element. In addition, each row or column in the multiplication table represents a set of h distinct matrix elements. The mean entropy of probability distribution of the matrix elements into a certain row or column, H_G^{row} or H_G^{column}, respectively, may also be specified by the Shannon's equation. Since the probability of an arbitrarily chosen matrix element being in one of the row (or column) subsets, $p_i = 1/h$, is the same as that of one row (or column) being in one of the subsets of the multiplication table, and taking into account eqn.(6), one obtains :

$$H_G^{MT} = H_G^{MT'} = H_G^{row} = H_G^{column} = \log_2 h \qquad (7)$$

Finally, a decomposition of the h^2 elements of the multiplication table can be carried out according to their symmetry in relation to the main diagonal of the table. The matrix elements set divides into subsets of two and one elements only. Let have m pairs of identical elements symmetrically placed on both sides of the main diagonal. Each one of the others $h^2 - 2m$ elements will form an individual subset. Here are included h diagonal elements, and the rest $(h^2 - h - 2m)/2$

pairs of different non-diagonal elements. Taking the probabilities of these two kinds of subsets $p_1 = 2/h$, and $p_2 = 1/h^2$, respectively, the mean entropy of this probability distribution, $H_G^{MT,D}$ can be specified :

$$H_G^{MT,D} = - m.2/h^2.\log_2 2/h^2 - (h^2-2m).1/h^2.\log_2 1/h^2 =$$

$$= \log_2 h^2 - 2m/h^2 \qquad (8)$$

More details concerning the statistical characteristics of the finite point groups of symmetry, introduced here on the basis of Information Theory, as well as equations characterizing each of the groups important to chemistry, will be published elsewhere. In this paper we centre our attention to the statistical properties of the finite point groups, specifying them in a number of theorems.

3. Theorems Concerning the Entropy Characteristics of Finite Point Groups

THEOREM 1. The isomorphic groups have the same mean entropy :

$$H_{G_1} = H_{G_2} \cong G_1 \qquad (9)$$

This theorem holds for the mean entropy of any kind of distribution of the symmetry elements in the group (into: classes, irreducible representations, subgroups, multiplication table, etc.). All these substructures of two isomorphic groups are identical since such groups belong to one and the same abstract group. Then, due to the same elements distribution, the probabilities in eqn.(1) will be the same and the two isomorphic groups will have the same mean entropy.

A theorem opposite to Theorem 1 does not hold. Two non-isomorphic groups may have the same mean entropy, especially when the order of the groups is small.

When one deals with the distribution of symmetry elements into the multiplication table of the group, the entropy equality extends to nonisomorphic groups as well :

THEOREM 2. The groups of equal order have the same mean entropy of the symmetry elements distribution into the multiplication table of the group and its rows and columns :

$$\text{if} \quad h_1 = h_2 = h_3 = \dots = h_k ,$$
$$H_{G_1} = H_{G_2} = H_{G_3} = \dots = H_{G_k} \qquad (10)$$

Here H_{G_i} is each one of the mean entropies introduced by eqns.(6,7) for the group having an order h_i. The proof of (10) follows immediately from eqns.(6,7), in which H_G quantities are expressed as a function of the order h only.

THEOREM 3. For a given order h the abelian groups have a maximum mean entropy of probability distributions on the classes of symmetry elements, as well as on the irreducible representations of the group, which is always greater than the corresponding mean entropies of the nonabelian groups.

$$H_G^{Cl(IR)}(\text{ABELIAN}) = \log_2 h = \max > H_G^{Cl(IR)}(\text{NONABELIAN}) \qquad (11)$$

Proof. Each element in the abelian groups forms a separate class. Since the number of the irreducible representations of the group is equal to the number of its classes of symmetry elements, all the irreducible representations in the abelian groups are one-dimensional. Then, in eqn.(3) $N_i=1$, and in eqn. (5) $l_i^2=1$. Thus, one obtains for both equations to equal the maximum mean entropy $H_{max} = \log_2 h$. There is at least one class having more than one element ($N_i > 1$), as well as at least one irreducible representation of a dimension higher than 1 ($l_i^2 > 1$) in the nonabelian groups. Then in that case the mean entropy is not maximum and the theorem is proved.

THEOREM 4. Among two groups of equal order, that group in which the classes of elements are more in number and with a smaller number of elements in them, has a higher mean entropy of probability distribution over the classes of symmetry elements:

$$H_G^{Cl(r)} > H_G^{Cl(k)} \quad , \ (h{=}const, \ r>k) \tag{12}$$

Here the number of classes in the two groups is denoted by r and k, respectively.

Proof. Let denote the number of elements in the classes of the first and second group by $N'_1, N'_2, \ldots, N'_r$, and $N''_1, N''_2, \ldots, N''_k$, respectively. Using eqn.(4), after some simple transformations one obtains :

$$\Delta H_G^{Cl} = H_G^{Cl(r)} - H_G^{Cl(k)} =$$

$$= \sum_{i=1}^{k<r} N''_i/h.\log_2 N''_i/h - \sum_{i=1}^{r} N'_i/h.\log_2 N'_i/h =$$

$$= 1/h\left(\sum_{i=1}^{k<r} N''_i.\log_2 N''_i - \sum_{i=1}^{r} N'_i.\log_2 N'_i\right) \tag{13}$$

There are always some $N'_i = N''_i$, including here the case i=1, $N'_1 = N''_1 = 1$, dealing with the identity elements of the two groups. By definition the first group has not only a larger number of classes, but also a smaller number of elements in them. The elements of the two groups can be ordered so that

$$N''_i > N'_i \quad (\text{for } i=1,2,3,\ldots,k<r)$$

An additional condition can be taken here that there is at least one N''_i which is a sum of two or several N'_i : $N''_i = \sum N'_i$. (This is always true for the point groups of small and moderate order which are of importance to chemistry. It is not known, however, if this equality holds always.). Given the above, and since

$$(x + y + z + \ldots).\log_2 (x + y + z + \ldots) > x.\log_2 x + y.\log_2 y + z.\log_2 z + \ldots$$

we obtain

$$\Delta H_G^{Cl} = 1/h(\sum N''_i.\log_2 \sum N''_i - \sum N'_i.\log_2 N'_i) > 0 \ ,$$

proving the inequality (12).

THEOREM 5. Among two groups of equal order, that group in which the irreducible representations are more in number and with a smaller dimension, has a larger mean entropy of probability distribution over the IR :

$$H_G^{IR(r)} > H_G^{IR(k)} \quad (h=\text{const}, \ r>k) \qquad (14)$$

Here the number of irreducible representations of the two groups is denoted by r and k, respectively.

Assigning the dimensions of the first and second group by $N'_1, N'_2, \ldots, N'_r$, and $N''_1, N''_2, \ldots, N''_k$, respectively, and making use of the decomposition of the group order h into a sum of the squares of the dimensions of IR (eqn.4) one obtains

$$H_G^{IR(r)} - H_G^{IR(k)} = 1/h\left(\sum_{i=1}^{k<r} N_i''^2 . \log_2 N_i''^2 - \sum_{i=1}^{r} N_i'^2 . \log_2 N_i'^2\right) \qquad (15)$$

Similarly to theorem 4, the inequality (14) proves under the restricted condition that at least one $N_i''^2$ is equal to the sum of two or several $N_i'^2$: $N_i''^2 = \sum N_i'^2$.

THEOREM 6. Let the integer h be partitioned into a sum of the integers N_i. There are always finite point groups with an order h which have the maximum mean entropy of probability distribution on the classes of N_i elements in the group. There are no groups having the minimum mean entropy.

Proof. For each finite h some abelian groups exist (C_n, S_n, etc.) containing h classes of one element. According to the theorem 3 they have a maximum mean entropy $H_G^{Cl} = \log_2 h$. These groups in which all the elements are in one class will contain a minimum mean entropy. $N_i = h$ in them, the probability $p_i = h/h = 1$, and $H_G^{Cl} = 0$. But the identity element E always forms a separate class. Therefore, in all the groups (except the trivial group C_1) $k>1$ and $N_i<h$, i.e. $H_G^{Cl} > H_{G,min}^{Cl} = 0$.

THEOREM 7. If different partitions of a given integer h, as a sum of the squares of the integers N_i are possible, then there are always such finite point groups of symmetry of order h, which contain a maximum mean entropy of probability distribution over the irreducible representations of N_i dimention in the group. There are no groups of zero mean entropy. Groups with a relative minimum of mean entropy exist rarely.

Proof. There are abelian groups (C_n, S_n, C_{nh}) for each finite h, which according to theorem 3 have a maximum mean entropy H_G^{IR}. Except the trivial group C_1, partitions having zero mean entropy, for example for $h = 4\ (2^2)$, $h = 9\ (3^2)$, $h = 16\ (4^2)$, etc., do not exist, since each group has at least one one-dimensional irreducible representation. Probability distributions having a possible minimum mean entropy H_G^{IR} do not always exist. They do not exist, for instance, for the groups having $h = 8\ (2^2 + 2^2)$, $h = 10\ (3^2 + 1^2)$, $h = 16\ (3^2 + 2^2 + 3.1^2)$, etc. For the group T of order h = 12, however, a partition to one three-dimensional and three one dimensional representations $(3^3 + 3.1^2)$ takes place, which carries a minimum entropy H_G^{IR}, as compared to the other possible partitions $(12.1^2;\ 8.1^2 + 2^2;\ 4.1^2 + 2.2^2)$.

THEOREM 8. Only such finite point groups of symmetry of odd order h exist, which have a maximum mean entropy of probability distribution over the classes of symmetry elements, as well as over the irreducible representations of the group.

Proof. The groups of odd order, including those having subgroups are always abelian. According to theorem 3 these groups have always the maximum mean entropy.

THEOREM 9. The finite point groups of symmetry, which do not have proper subgroups (the so called simple groups), always have the maximum mean entropy of probability distribution over the classes of symmetry elements, as well as over the irreducible representations of the group.

Proof. According to the theorem of Lagrange, the order of a finite group is divisible by the order of each of its subgroups. Then, if the order of the group is a prime number, the group has no proper subgroups. Theorem 8 holds for the odd prime numbers. For the unique even prime number h = 2, there exists a unique partition ($2 = 1^2 + 1^2$), which carries a maximum entropy (eqn.5). Hence the theorem is proved.

THEOREM 10. The mean entropies of probability distributions of the matrix elements in the multiplication table of the group, of the matrix elements in a row or column of the table, as well as of the rows (or columns) in the group, are equal.

The theorem is expressed by eqn.(7) and proved there.

The statistical property of the point groups of symmetry, expressed by theorem 10, is a specific result for a group multiplication table. In arbitrary h x h matrix, the mean entropy of elements distribution in a given row (or column) in the general case is not equal to the mean entropy of elements distribution in the whole matrix. This follows from the fact, that when all the matrix elements are included in a common set, a union of these elements into joint sets of equal elements takes place. This results in a different mean entropy of the matrix and the rows (or columns) in it.

THEOREM 11. The mean entropy of probability distribution of the matrix elements in the multiplication table of a finite point group is exactly half of the maximum mean entropy of a square matrix of the same h x h size, dividing into two equal parts the total interval of values, in which the mean entropy of such matrices is defined :

$$H_G^{MT} = \log_2 h = \tfrac{1}{2}.H_{MATR}^{max} \qquad (16)$$

$$0 \le H_{MATR} \le \log_2 h^2 \qquad (17)$$

The equation (17) was preliminarily obtained[18] for an arbitrary square h x h matrix, the mean entropy in which is zero when all the matrix elements are the same, and conversly, it is a maximum one when all the matrix elements are distinct. The proof of eqn.(16) follows from the comparison of equations (6) and (17).

THEOREM 12. The finite point abelian groups have less mean entropy of the matrix elements distribution symmetrically in relation to the main diagonal of the multiplication table, than the nonabelian :

$$H_G^{MT,D}\ (\text{ABELIAN}) < H_G^{MT,D}\ (\text{NONABELIAN}) \qquad (18)$$

Proof. Equation (8) derived earlier refers to the nonabelian groups. In the case of the abelian groups all symmetry elements of the group commute. Then the number of pairs of identical elements will be equal to half of the all non-diagonal elements :

$$m' = \tfrac{1}{2}(h^2 - h) > m$$

Hence, the second term in eqn.(8) will increase, and the mean entropy will be smaller for the abelian groups.

4. Theorems Concerning the Change in the Entropy Characteristics of Finite Point Groups

The molecules of different chemical compounds often reduce their symmetry when affected by various factors. This occurs for instance in the case of substitution reactions, molecular vibrations, as a consequence of the effect of Jan-Teller, etc. Accordingly, it is of interest to study the change in the mean entropy of probability distributions, introduced for the finite point groups by eqns.(3-8), when transition to one of their subgroups has taken place.

THEOREM 13. When a group reduces its symmetry to that of its subsubgroup, the change in the mean entropy of each one of probability distributions of symmetry elements is determined additively from the change of these quantities for the transitions group-subgroup (G-SG) and subgroup-subsubgroup (SG-SSG) :

$$\Delta H_{G-SSG} = \Delta H_{G-SG} + \Delta H_{SG-SSG} \qquad (19)$$

Proof.

$$\Delta H_{G-SSG} = H_G - H_{SSG} = (H_G - H_{SG}) + (H_{SG} - H_{SSG}) =$$

$$= \Delta H_{G-SG} + \Delta H_{SG-SSG}$$

Since the proof does not depend on the type of entropy measure, it holds for all quantities introduced by eqns.(3-8).

<u>THEOREM 14</u>. The change in the mean entropy of probability distribution over the classes of symmetry elements, when the symmetry of C_{nv} group reduces to C_n, as well as when D_{nh} group reduces to C_{nh}, is greater for even, than for odd order of the main rotation axis n :

$$\Delta H^{Cl}_{C^O_{(n-1)v}-C^O_{n-1}} < \Delta H^{Cl}_{C^E_{nv}-C^E_n} > \Delta H^{Cl}_{C^O_{(n+1)v}-C^O_{n+1}} \qquad (20)$$

$$\Delta H^{Cl}_{D^O_{(n-1)h}-C^O_{(n-1)h}} < \Delta H^{Cl}_{D^E_{nh}-C^E_{nh}} > \Delta H^{Cl}_{D^O_{(n+1)h}-C^O_{(n+1)h}} \qquad (21)$$

<u>Proof :</u>

a) <u>C_{nv}-C_n case</u>. Expressing the mean entropy of the groups under consideration as a function of their order, the following equations can be derived :

$$\Delta H_{C^E_{n_v}-C_n} = 1 + 2/h \ , \quad \Delta H_{C^O_{nv}-C_n} = \tfrac{1}{2} + 1/h' \qquad (22)$$

The order h' of the group C_{nv} for an odd n is smaller or greater, than the order h of the same group at n even, by two units ($h' = h-2$, and $h' = h+2$). Subtracting the two eqns.(22) and substituting h, we obtain :

$$\text{for } h' = h - 2 \ , \quad \Delta H_{E/O} = \tfrac{1}{2} + 2/h > 0 \qquad (23)$$

$$\text{for } h' = h + 2 \ , \quad \Delta H_{E/O} = \tfrac{1}{2} > 0 \qquad (24)$$

Thus the inequality (20) is proved.

b) <u>D_{nh}-C_{nh} case</u>. Analogically

$$\Delta H_{D^E_{nh}-C_{nh}} = 3/2 + 4/h \ ; \quad \Delta H_{D^O_{nh}-C_{nh}} = 1 + 2/h' \qquad (25)$$

$$\text{for } h' = h - 2 , \quad \Delta H_{E/O} = \tfrac{1}{2} + 6 > 0 \tag{26}$$

$$\text{for } h' = h + 2 , \quad \Delta H_{E/O} = \tfrac{1}{2} - 2/h > 0 \tag{27}$$

In the last case the inequality (27) holds for each h, since the minimum order of D_{nh} group is h = 8 (D_{2h} group).

Theorem 14 expresses an interesting feature of the mean entropy of elements distribution over the classes in the C_{nv} and D_{nh} groups - its different manner of changing at even and odd order of the main rotation axis n. This result recalls the different change in the properties of n-alkanes, containing an even and odd number of carbon atoms and eventually it could be a basis for some correlations.

THEOREM 15. The mean entropy of the elements distribution in the multiplication table of the group, as well as over its rows (or columns), reduces by 1 bit in transitions from a group to a subgroup which has an order half as large:

$$\Delta H^{MT}_{G-SG} = \Delta H^{row}_{G-SG} = \Delta H^{column}_{G-SG} = 1 \text{ bit} , \text{ if } g = h/2 \tag{28}$$

Eqn.(28) follows immediately from eqn.(7) and the condition $g = h/2$. The physical essence of this result is that the uncertainty of matrix elements distribution decreases exactly twice when a reduction in symmetry of the group of order h to its subgroup of order $g = h/2$ takes place.

THEOREM 16. The mean entropy of the matrix elements distribution in the multiplication table of a finite point group is an additive quantity equal to the sum of the mean entropy of any of its subgroups and the logarithm at a basis two of the quotient of the orders of the two groups:

$$H^{MT}_{G} = H^{MT}_{SG} + \log_2 a \tag{29}$$

Proof. Let a finite point group has an order h. Let a subgroup of this group has an order $g = h/a$. Then according to eqn.(7)

$$H_G^{MT} - H_{SG}^{MT} = \log_2 h - \log_2 h/a = \log_2 a \ ,$$

which proves eqn.(29).

Theorem 16 holds for each of the entropy characteristics of the multiplication table of the group, introduced by eqn. (7).

When a homomorphism of the group onto the subgroup exists the quotient a from eqn.(29) expresses the homomorphic ratio ($h : g = a : 1$). Additionally, the case $a = 1$ occurs for the trivial subgroup having an order $g = h$, as well as a mean entropy equal to that of the group. Thus, theorem 16 dealing with the homomorphic correspondence between two groups contains as a specific case ($a=1$) the theorem on the equal mean entropy of two isomorphic groups (theorem 1).

THEOREM 17. The mean entropy of probability distribution over the irreducible representations of a finite point group is a semiadditive function of the mean entropy of the subgroup and the quotient of the orders of the two groups :

$$H_G^{IR} = H_{SG}^{IR} + \log_2 a + \Delta \qquad (30)$$

The correction for semiadditivity Δ is a simple function of the order of the subgroup and has a different value for most subgroups. $\Delta = 0$ for the cases $C_{2n}-C_n$, $C_{2nh}-C_{nh}$, $C_{nh}-C_n$, $D^O_{nd}-D_n$, $C^O_{2nv}-C_{nv}$, $D^E_{nh}-C^E_{nv}$, $D^E_{nh}-D_n$, O_h-O, et al. Some examples follow where $\Delta \neq 0$:

$C^O_{nv}-C_n$, $\Delta = 4/h$; $C^E_{nv}-C_n$, $\Delta = 8/h$; $D^E_{nh}-C_{nh}$, $\Delta = 16/h$, etc.

5. Entropy Relation for Direct Products of Finite Point Groups

Let a direct product of two groups G_1 and G_2, having an order h_1 and h_2, respectively, be considered. Let also the set of symmetry elements in each of the two groups be partitioned according to a certain structural criterion to k and m subsets: $N'_1, N'_2, \ldots, N'_k$, and $N''_1, N''_2, \ldots, N''_m$. The probability distributions associated with the two groups will be $p'_1, p'_2, \ldots, p'_k$, and

$p''_1, p''_2, \ldots, p''_m$, respectively. The group $G_1 \times G_2$, called a direct product of G_1 and G_2, has an order $h_1 \times h_2$. The set of its elements, $N_1, N_2, \ldots, N_{km}$, is composed of the products of each element of the group G_1 and all the elements of the G_2 group. The probability distribution associated with this group will be $p_1, p_2, \ldots, p_{km}$, where each one of the probabilities p_i equals the product of one probability of the first group and one probability of the second group :

$$p_i = p'_j \cdot p''_l \tag{31}$$

The following theorem holds:

<u>THEOREM 18</u>. The mean entropy of any kind of probability distributions, associated with a finite point group, which is a direct product of two groups is equal to the sum of the corresponding mean entropies of the two groups:

$$H_{G_1 \times G_2} = H_{G_1} + H_{G_2} \tag{32}$$

<u>Proof</u>. According eqn.(1) the mean entropies of the three groups are, respectively :

$$H_{G_1} = - \sum_{j=1}^{k} p'_j \cdot \log_2 p'_j \tag{33}$$

$$H_{G_2} = - \sum_{l=1}^{m} p''_l \cdot \log_2 p''_l \tag{34}$$

$$H_{G_1 x G_2} = - \sum_{i=1}^{k.m} p_i \cdot \log_2 p_i \tag{35}$$

Introducing eqn.(31) in (35) one obtains

$$H_{G_1 x G_2} = - \sum_{j=1}^{k} \sum_{l=1}^{m} p'_j \cdot p''_l \cdot \log_2 p'_j p''_l =$$

$$= - \sum_{j=1}^{k} p'_j \sum_{l=1}^{m} p''_l \cdot \log_2 p''_l - \sum_{l=1}^{m} p''_l \cdot \sum_{j=1}^{k} p'_j \cdot \log_2 p'_j$$

Since $\sum_{j=1}^{k} p'_j = 1$, and $\sum_{l=1}^{m} p''_l = 1$, and taking into account eqns.(33) and (34), the theorem is proved.

Theorem 18 holds for each of the entropy characteristics of the finite point groups, introduced by eqns.(3-8), since the proof of this theorem does not depend on the kind of probability distribution.

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