Investigation of matrix representation of complex compound with help of group theory and symmetry

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ABSTRACT

In this paper we have studied the matrix representation and symmetry of complex with the help of Group theory. Group theory provides a formal means for exploiting symmetry in the analysis of physical system. The symmetry of molecules and solids is a very powerful tool for developing and understanding the bonding and its physical properties. A complex is prepared by the interaction of phthallic acid and di-tertiary amyl chromate in suitable solvent. The properties of character tables are presented and the method for obtaining a matrix representation for all the motions of a complex is detailed.

Keywords: Point group, irreducible representation, Character table, wave function.

INTRODUCTION

According to the Schrödinger wave equation for any physical system i.e. $H\psi_j=E_j\psi_j$ where H is the Hamiltonian operator, which indicates that certain operations are to be carried out on the state function ψ. The Hamiltonian operator is obtained by writing the expression for the classical energy of the system, which is simply the sum of the potential and kinetic energies for the system of interest to us, and then replacing the momentum terms by differential operators according to the postulates of wave mechanics. Each Eigen function is associated with a certain energy level E_j. Therefore, molecular Eigen functions and energy levels can be labeled with a symmetry index jwhich indicates the point symmetry group of the molecule. The quantitative characteristic of the labeling is a character table which shows the behavior of the molecular wave functions under the symmetry operations of the molecular symmetry point group. Since only certain combinations of symmetry elements occur in the various point groups and since some of their symmetry elements are consequence of others, only certain combinations of symmetry properties of the vibrational (and electronic) wave functions are possible. In the molecular spectroscopy these combinations of symmetry properties are called symmetry types, or species. In the formal group theory the same combinations are called irreducible representations of the group.

We use in this paper the following ideas of group representation:

We discuss below any reducible representation of a group and irreducible ones of that group which of pivotal importance .The character of a matrix which represents the group is the sum of all its diagonal elements (also called trace of the matrix).We know that for any reducible representation it is possible to find some similarity transformation which will reduce each matrix to one consisting of block along the diagonal, each of which belongs to an irreducible representation of the group. We also know that the character of a matrix is not changed by the similarity transformation. Thus we express χ(G(gj)), the character of the matrix G corresponding to the operation g_j in a reducible representation as follows,

$$\chi\,(G(g_j)\,) = \Sigma a_j\,\chi\,(G(g_j))\;.\;\ldots\ldots\ldots\ldots(A)$$

where a_j represent the number of times the block constituting the jth irreducible representation will appear along the diagonal when the reducible representation is completely reduced by the necessary similarity transformation. Now multiply each side of eq. (A) by $\chi\,(G(g_i))$ and then sum each side all operations namely ,

$$\Sigma_g\,\chi\,(G(g_j))\chi\,(G(g_i) \quad = \Sigma_g\Sigma_j\,a_j\,\chi\,(G(g_j))\chi\,(G(g_i))$$

$$= \Sigma_{\,j}\,\Sigma_g\,\chi\,(G(g_j))\chi\,(G(g_i))$$

Now for each terms in the sum over j ,we have

$$\Sigma_g\,a_j\,\chi\,(G(g_j))\chi\,(G(g_i)) \;=\; a_{\,j}\Sigma_g\,\chi\,(G(g_j))\chi\,(G(g_i)) \;= a_j\,n\,\delta_{ij}$$

MATERIAL AND METHOD

In this paper group of symmetries of Penta aqua phallate chromium (I) complex is studied. The character table of the group is computed. The dimensionality of the irreducible representation of the group can be determined by a simple rule which state that the sum of the squares of the dimension of the representations equals the order of the group (order of the group is the number of its elements).When matrices G(g) are given, it is useful to be recognize whether the representation is irreducible if following conditions is satisfied :

$$\Sigma_g\,\chi(G(g)) * \chi(G(g)) \;= n$$

Where χ(G(g)) is the character of the group element g [trace of the matrix G(g)].Irreducible representations also satisfy two orthogonality[3] relations:

$$\Sigma_g\,\chi(G(g_i)) * \chi(G(g_j)) = n\,\delta_{ij}$$

$$\Sigma_g \chi(G(g_j)) * \chi(G(g_k)) = n\, \delta_{jk}.$$

We use different experimental facts to obtain the structure of complex **[Cr ($C_8H_5O_4$) (H_2O) $_5$]** which is a square planer and it is of C_{4v} group. Its elements are E, C_4, $C^2_4 = C^2$, C^3_4, σ_v, σ'_v, σ_d, σ'_d where

E = The identity , C_4 = A clockwise rotation through 90, C^2_4 = A clockwise rotation through 180

C^3_4 = A clockwise rotation through 270, σ_v = Reflection in line x-axis. σ'_v = Reflection in line y-axis

σ_d = Reflection in line y = x & σ'_d = Reflection in line y = -x

Illustration of five theorems used:

1.The number of irreducible representations is equal to the number of conjugate classes[4] in the group.

The symmetry operations in C_{4v} point group are: E, C_4, $C^2_4 = C^2$, C^3_4, σ_v, σ'_v, σ_d, σ'_d.

There are five classes of symmetry operations derived using a multiplication table:

	E	C_4	C^2_4	C^3_4	σ_v	σ'_v	σ_d	σ'_d
E	E	C_4	C^2_4	C^3_4	σ_v	σ'_v	σ_d	σ'_d
C^3_4	C^3_4	E	C_4	C^2_4	σ'_d	σ_d	σ_v	σ'_v
C^2_4	C^2_4	C^3_4	E	C_4	σ'_v	σ_v	σ'_d	σ_d
C_4	C_4	C^2_4	C^3_4	E	σ_d	σ'_d	σ'_v	σ_v
σ_v	σ_v	σ'_d	σ'_v	σ_d	E	C^2_4	C^3_4	C_4
σ'_v	σ'_v	σ_d	σ_v	σ'_d	C^2_4	E	C_4	C^3_4
σ_d	σ_d	σ_v	σ'_d	σ'_v	C_4	C^3_4	E	C^2_4
σ'_d	σ'_d	σ'_v	σ_d	σ_v	C^3_4	C_4	C^2_4	E

[E], [C^2_4], [C_4,C^3_4], [σ_v,σ'_v], and [σ_d,σ'_d], i.e. there will be five irreducible representations .

2) The characters[5] of all operations in the same class are equal in each given irreducible (or reducible) representation.

In above example, all rotations of C_4, C^3_4 will have the same character; all mirror planes

σ_v, σ'_v, σ_d , σ'_d will have the same character, etc.

3) The sum of the squares of all characters in any irreducible representation is equal to the order of the group.

The character table for C_{4v} is

	E	C_4	C^2_4	C^3_4	σ_v	σ'_v	σ_d	σ'_d
A_1	1	1	1	1	1	1	1	1
A_2	1	1	1	1	-1	-1	-1	-1
B_1	1	-1	-1	1	-1	-1	1	1
B_2	1	-1	-1	1	1	1	-1	-1
E	2	0	0	-2	0	0	0	0

Here A_1: $1^2 + 1^2 + 1^2 + 1^2 + 1^2 + 1^2 + 1^2 + 1^2 = 8$ = order of group.

A_2: $1^2 + 1^2 + 1^2 + 1^2 + (-1)^2 + (-1)^2 + (-1)^2 + (-1)^2 = 8$= order of group.

B_1: $1^2 + (-1)^2 + (-1)^2 + 1^2 + (-1)^2 + (-1)^2 + 1^2 + 1^2 = 8$= order of group.

4) The point product of the characters of any two irreducible representations is 0.

From above table for C_{4v}

$\Gamma A_1 * \Gamma A_2 = (1*1) + (1*1) + (1*1) + (1*1) + (1*-1) + (1*-1) + (1*-1) + (1*-1) = 0$

$\Gamma A_1 * \Gamma B_1 = (1*1) + (1*-1) + (1*-1) + (1*1) + (1*-1) + (1*-1) + (1*1) + (1*1) = 0$

$\Gamma A_1 * \Gamma E = (1*2) + (1*0) + (1*0) + (1*-2) + (1*0) + (1*0) + (1*0) + (1*0) = 0$

Similarly we can obtained other results.

This shows that all irreducible representations are orthogonal.

5) The sum of the squares of the dimensions of the irreducible representations is equal to the order of the group.

In the point group C_{4v} the irreducible representation

A_1 is 1 dimensional

A_2 is 1 dimensional

B_1 is 1 dimensional

B_2 is 1 dimensional

E is 2 dimensional.

The order of the group is $8 = 1^2+1^2+1^2+1^2+2^2$.

The matrix representation of all the symmetry operations in C_{4v} is

$$E = \begin{bmatrix} \cos 0 & -\sin 0 & 0 \\ \sin 0 & \cos 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = I_{3\times3}$$

$$C_4^1 = \begin{bmatrix} \cos {}^{\pi}/_{2} & -\sin {}^{\pi}/_{2} & 0 \\ \sin {}^{\pi}/_{2} & \cos {}^{\pi}/_{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad C_4^2 = \begin{bmatrix} \cos \pi & -\sin \pi & 0 \\ \sin \pi & \cos \pi & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$C_4^3 = \begin{bmatrix} \cos {}^{3\pi}/_{2} & -\sin {}^{3\pi}/_{2} & 0 \\ \sin {}^{3\pi}/_{2} & \cos {}^{3\pi}/_{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \sigma_v = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\sigma_v' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \sigma_d = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \ \& \ \sigma'_d = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

CONCLUSION: Each individual matrix is called a representative of the corresponding symmetry operation, and the complete set of matrices is called a matrix representation of the group. The matrix representative's act on some chosen basis set of functions, and the actual matrices making up a given representation will depend on the basis that has been chosen. The representation is then said to span the chosen basis.

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