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# On the Character and Conjugacy Classes of $C_{3v}$ Point Group Using Block Diagonal Matrix

**David Terna Achaku[1], Moses Anayo Mbah[2], Peter Vanenchii Ayoo[3]**

Department of Mathematics, Federal University Lafia, P.M.B 146 Lafia, Nigeria

**Abstract:** ***Using the transformation of the symmetry elements of $C_{3v}$ point groups, we constructed their matrix representation, applying the orthogonality theorem, we reduced the blocked diagonal matrix to its irreducible form to get the character table. The character table thus showed the three conjugacy classes.***

**Keyword**: Conjugacy Classes, Point Groups, Orthogonality, Character Table, Irreducible, Symmetry Elements.

## 1. Introduction

The classification of molecules according to their point groups, provides a rigorous method for predicting optical activities. For a molecule to exhibit optical activity, it must belong to a point group that does not posses an inversion centre,mirror plane or improper rotation[1]. Though it is possible to reduce an element or molecule to an optical active type. As seen in Zincblende-type semiconductors, which is a $Td$. The $60d$ reflection planes present in this group forbid optical rotatary power (Circular birefringence and dichroisin)[2]. Under static uniaxial stress along one of the $S_4$ axis $T_d$ is reduced to $D_{2d}$ and as such circular birefringence and dichroisin become allowed by [3] optical activity (i.e the existence of two different indices of refraction for right or left circularly polarized light is impossible in crystals with a centre of inversion by [4].

In group theory, a dihedral group is the group of symmetries of a regular polygon, including both rotations and reflections. In geometry the group is denoted by $D_n$, while in algebra the same group is denoted by $D_{2n}$. Coxetor rotation denotes the reflectional dihedral symmetry as $[n]$ order $2n$ and rotational dihedral symmetry as $[n]^+$ order $n$. Orbifold rotation gives the reflective symmetry as $^+nn$ and rotational as $n$ [5]. In this paper we shall denote it as $D_{2n}$, the symmetries of a regular polygon with $n$ sides.

## 2. Group Structure of $D_{2n}$

The composition of two symmetries of a regular polygon is again symmetry. It is the result of this operation that gives the symmetries of a regular polygon the result of a finite group [5]. It is non-abelian and include point groups known as $C_{3h}$, $C_{3v}$ and $S_3$. $D_6$ is the symmetry group of the equilateral triangle. $D_{2n}$ has the following elements [5].

$$D_{2n} = \{\gamma_0 = e, \gamma_1, \gamma_2, ..., \gamma_{n-1}, f_0, f_1, ..., f_{n-1}\}$$

Such that

$$\gamma_i \gamma_j = \gamma_{(i+j)modn}; f_i f_j = f_{(i-j)modn}, f_i f_j = \gamma_{(i-j)modn}$$

The $2n$ elements of $D_{2n}$ can be written as $e, \gamma, \gamma^2, ..., \gamma^{n-1}; f, \gamma f, \gamma^2 f, ..., \gamma^{n-1} f$. The first $n$ elements are the elements of the rotation while the remaining are those of the reflection and so we write.

$$D_{2n} = \{\gamma, f \mid \gamma^n = e = f^2, f\gamma f = \gamma^{-1}, \gamma f \gamma = f, \gamma^2 = f^2 = \gamma f = e\}$$

**Theorem 2.1**

Conjugacy classes of the Dihedral group
$D_{2n} = <\gamma, \rho : \gamma^2 = \rho^n = 1, \rho\gamma = \gamma\rho^{-1}>$

**Proof**

First we compute the conjugacy class of a rotation $\rho^k$. If we conjugate it by some $\rho^i$, then we get $\rho^i \rho^k \rho^{-i} = \rho^k$, which gives us nothing new. If we conjugate it by some $\gamma\rho^i$ then we get

$$\begin{aligned} \gamma\rho^i \rho^k (\gamma\rho^i)^{-i} &= \gamma\rho^i \rho^k \rho^{-i} \gamma \\ &= \gamma\rho^k \gamma \\ &= \gamma\gamma\rho^{-k} \\ &= \rho^{-k} \end{aligned}$$

Hence the conjugacy class of $\rho^k$ consists of $\{\rho^k, \rho^{-k}\}$. Rotation occurs in inverse pairs. If $n$ is odd then the set $\{1, \rho, ..., \rho^{n-1}\}$ breaks into classes $\{1\}$ and $\left\{\rho^{\frac{n}{2}}\right\}$, together with pairs $\{\rho^i, \rho^{-i}\}$ for $i = 1 ... \frac{n-2}{2}$.

Next we compute the conjugacy classes of a reflection $\gamma\rho^k$. If we conjugate by some $\rho^i$ we get $\rho^i\gamma\rho^k\rho^{-1} = \gamma\rho^{-1}\rho^k\rho^{-i} = \gamma\rho^{k-2i}$. But if we conjugate by some $\gamma\rho^i$ (move all copies of $\gamma$ to the left) we get

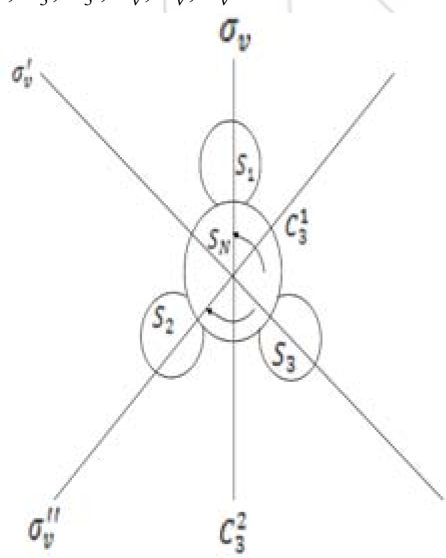
$$\gamma\rho^i\gamma\rho^k(\gamma\rho^i)^{-1} = \gamma\rho^i\gamma\rho^k\rho^{-i}\gamma$$
$$= \gamma\gamma\gamma\rho^i\rho^k\rho^i$$
$$= \gamma\rho^{2i-k}.$$

That is, the conjugacy class of $\gamma\rho^k$ consists of $\{\gamma\rho^{k-2i} : i \in Z\}$. If $n$ is odd, all of the reflections form a single conjugacy class but, if $n$ is even then the reflections break into two classes:

$$\{\gamma, \gamma\rho^2, \gamma\rho^4, ..., \gamma\rho^{n-2}\} \text{and} \quad \{\gamma\rho, \gamma\rho^3, ..., \gamma\rho^{n-1}\}.$$

A matrix representation of the $C_{3v}$ point group (ammonia molecule $NH_3$) The first thing to do is to choose a basis $(S_N, S_1, S_2, S_3)$ that consists of the valence $S$ orbitals on the nitrogen and the three hydrogen atoms and consider what happens to the basis when it is acted upon by each of the symmetry operations in the $C_{3v}$ point group with symmetry operations as

$$E, C_3^1, C_3^2, \sigma_v, \sigma_v^{'}, \sigma_v^{''}$$




The effects of the symmetry operations is as follows:

$$E \quad (S_N, S_1, S_2, S_3) \rightarrow (S_N, S_1, S_2, S_3)$$
$$C_3^1 \quad (S_N, S_1, S_2, S_3) \rightarrow (S_N, S_2, S_3, S_1)$$
$$C_3^2 \quad (S_N, S_1, S_2, S_3) \rightarrow (S_N, S_3, S_1, S_2)$$
$$\sigma_v \quad (S_N, S_1, S_2, S_3) \rightarrow (S_N, S_1, S_3, S_2)$$
$$\sigma_v^{'} \quad (S_N, S_1, S_2, S_3) \rightarrow (S_N, S_2, S_1, S_3)$$
$$\sigma_v^{''} \quad (S_N, S_1, S_2, S_3) \rightarrow (S_N, S_3, S_2, S_1)$$

Their equivalent matrices are

$$\Gamma(E) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \Gamma(C_3^1) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\Gamma(C_3^2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

$$\Gamma(\sigma_v) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\Gamma(\sigma_v^{'}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\Gamma(\sigma_v^{''}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

These symmetry operations form a group as is visible in the cayley table below. This is confirmed by simple matrix multiplication with the row matrices first.

**Table 1:** Cayley table

| | **E** | $C_3^1$ | $C_3^2$ | $\sigma_v$ | $\sigma_v^{'}$ | $\sigma_v^{''}$ |
|---|---|---|---|---|---|---|
| **E** | E | $C_3^1$ | $C_3^2$ | $\sigma_v$ | $\sigma_v^{'}$ | $\sigma_v^{''}$ |
| $C_3^1$ | $C_3^1$ | $C_3^2$ | E | $\sigma_v^{'}$ | $\sigma_v^{''}$ | $\sigma_v$ |
| $C_3^2$ | $C_3^2$ | E | $C_3^1$ | $\sigma_v^{''}$ | $\sigma_v$ | $\sigma_v^{'}$ |
| $\sigma_v$ | $\sigma_v$ | $\sigma_v^{''}$ | $\sigma_v^{'}$ | E | $C_3^2$ | $C_3^1$ |
| $\sigma_v^{'}$ | $\sigma_v^{'}$ | $\sigma_v$ | $\sigma_v^{''}$ | $C_3^1$ | E | $C_3^2$ |
| $\sigma_v^{''}$ | $\sigma_v^{''}$ | $\sigma_v^{'}$ | $\sigma_v$ | $C_3^2$ | $C_3^1$ | E |

From the definition of conjugacy classes above, it can be verified that

$$(C_3^1)C_3^2(C_3^1)^{-1}=\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&0&0&1\\0&1&0&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{pmatrix}$$

$$=\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{pmatrix}=C_3^1$$

The conjugacy classes are $\{E\}$, $\{C_3^1, C_3^2\}$ and $\{\sigma_v, \sigma_v^{'}, \sigma_v^{''}\}$

## 3. Reduction of matrix representations

Let us go back at $NH_3$ representation, and a careful observation shows that they all take the same block diagonal form.

$$\Gamma(E)\qquad \Gamma(C_3^1)\qquad \Gamma(C_3^2)$$

$$\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&0&0&1\\0&1&0&0\end{pmatrix}$$

$$\chi(E)=4\qquad \chi(C_3^1)=1\qquad \chi(C_3^2)=1$$

$$\Gamma(\sigma_v)\qquad \Gamma(\sigma_v^{'})\qquad \Gamma(\sigma_v^{''})$$

$$\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix},\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{pmatrix},\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&0&1&0\\0&1&0&0\end{pmatrix}$$

$$\chi(\sigma_v)=2\qquad \chi(\sigma_v^{'})=2\qquad \chi(\sigma_v^{''})=2$$

They can be written as a direct sum of a $|x|$ matrix and $3\times 3$ matrix as; with superscripts as $\Gamma^{(4)}(g)=\Gamma^{(1)}(g)\oplus\Gamma^{(3)}(g)$ dimension. The two reduced dimensions are displayed below

| $g$ | $E$ | $C_3^1$ | $C_3^2$ | $\sigma_v$ | $\sigma_v^{'}$ | $\sigma_v^{''}$ |
|---|---|---|---|---|---|---|
| $\Gamma^{(1)}(g)$ | $(1)$ | $(1)$ | $(1)$ | $(1)$ | $(1)$ | $(1)$ |

$1D$ rept span $(S_N)$

$$\Gamma^{(3)}(g)\quad \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$$

$$\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix}$$

$3D$ rep spanned by $S_1, S_2, S_3$

Note that $\Gamma^{(3)}(g)$ is not reducible since not all of the matrices are in block form, so applying a similarity transform with new basis, $S_1^{'}=\frac{1}{\sqrt{3}}(S_1+S_2+S_3)$, $S_2^{'}=\frac{1}{\sqrt{6}}(S_1-S_2-S_3)$ and $S_3^{'}=\frac{1}{\sqrt{2}}(S_2-S_3)$ or in matrix form

$$\underset{X'}{(S_1^{'},S_2^{'},S_3^{'})}=\underset{X}{(S_1,S_2,S_3)}\underset{C}{\begin{pmatrix}\frac{1}{\sqrt{3}}&\frac{2}{\sqrt{6}}&0\\\frac{1}{\sqrt{3}}&\frac{-1}{\sqrt{6}}&\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{3}}&\frac{-1}{\sqrt{6}}&\frac{-1}{\sqrt{2}}\end{pmatrix}}$$

From $\Gamma^{'}(g)=C^{-1}\Gamma(g)C$ we have

$$E\qquad C_3^1\qquad C_3^2\qquad \sigma_v\qquad \sigma_v^{'}\qquad \sigma_v^{''}$$

$\Gamma^{(3)}(g)$

$$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&0&0\\0&\frac{-1}{\sqrt{2}}&\frac{\sqrt{3}}{2}\\0&\frac{-\sqrt{3}}{2}&\frac{-1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}1&0&0\\0&\frac{-1}{\sqrt{2}}&\frac{-\sqrt{3}}{2}\\0&\frac{\sqrt{3}}{2}&\frac{-1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}\begin{pmatrix}1&0&0\\0&\frac{-1}{\sqrt{2}}&\frac{\sqrt{3}}{2}\\0&\frac{\sqrt{3}}{2}&\frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}1&0&0\\0&\frac{-1}{\sqrt{2}}&\frac{-\sqrt{3}}{2}\\0&\frac{-\sqrt{3}}{2}&\frac{1}{\sqrt{2}}\end{pmatrix}$$

So the reduced form of the $4$ dimensional derivation is

| $E$ | $C_3^1$ | $C_3^2$ | $\sigma_v$ | $\sigma_v^{'}$ | $\sigma_v^{''}$ |
|---|---|---|---|---|---|
| $(1)$ | $(1)$ | $(1)$ | $(1)$ | $(1)$ | $(1)$ |

$1$ dim span $=S_N$

| | | | | | |
|---|---|---|---|---|---|
| $(1)$ | $(1)$ | $(1)$ | $(1)$ | $(1)$ | $(1)$ |

$1$ dim span $=S_1^{'}$

$$\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}\frac{-1}{\sqrt{2}}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}\frac{-1}{\sqrt{2}}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}\frac{-1}{\sqrt{2}}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}\frac{-1}{\sqrt{2}}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{\sqrt{2}}\end{pmatrix}$$

$2$ dim span $=S_2^{'},S_3^{'}$

Irreducible representations and symmetry species, the two one-dimensional irreducible representations spanned by $S_N$

and $S_1^{'}$ are identical because they have the same symmetry, transforming in the same way under all of the symmetry operations of the point group.

Thus the one-dimensional irreducible representation (irrep)is symmetric with character $+1$ with rotation $A_1$ under all the symmetry operations of $C_{3v}$ while the $2-$dimensional irrep has character $2$ under the identity operation, $-1$ under rotation and $0$ under reflection and belongs to the irrep $E$.

$C_{3v}$ character table. The character table of $C_{3v}$ is shown below,

| $C_{3v},3m$ | $E$ | $2C_3$ | $3\sigma_v$ | $H=6$ |
|---|---|---|---|---|
| $A_1$ | $1$ | $1$ | $1$ | $z, z^2, x^2+y^2$ |
| $A_2$ | $1$ | $1$ | $-1$ | $R_z$ |
| $E$ | $2$ | $-1$ | $0$ | $(x,y),(xy,x^2+y^2),(xz,yz),(R_x,R_y)$ |

## 4. Discussion

The fuctions in the last column of the character table are important in many chemical applications of group theory especially in spectroscopy. By looking at the last column, we discover the symmetry of translations along the $x, y$ and $z$ axes. Since they determine whether or not a molecule can absorb a photon of $x-, y-$ or $z-$ polarised light and under a spectroscopic transition.

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