Group Theory and Character Tables

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Notes largely follow Albert F. Cotton, *Chemical Applications of Group Theory*, Ch 4

Representation Theory

How do we represent reality?
There is the "reality" and there is the representation of that "reality".

- For example, consider $\boxed{\text{Ten}}$, the number.

o o o o o o o o o o	← "ten" "things". (what is a "thing" anyway?)
TEN or ten	← In english.
10	← in hindu-arabic numerals. in base 10
दस , dias	← Hindi / Spanish
11	← in base 9
1010	← in base 2
11110	← in base (-2)

- All of the above "represent" the same idea but different ways of "representing" them.

- Vectors – example:

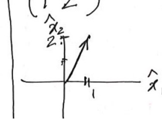
$1\hat{x}_1 + 2\hat{x}_2$

$(\hat{x}_1, \hat{x}_2) = (1, 2)$

$1 + i2$

$\begin{pmatrix} 1 \\ 2 \end{pmatrix}$

$(1, 2)$

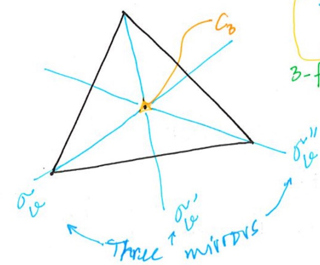


A Group

Is a **SET** that has **four** requirements:

1. Should be closed under the group operation
2. Should have identity as an element
3. Every element should have an inverse
4. Associativity

Example :



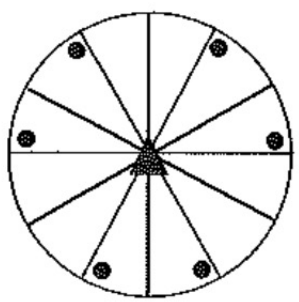
name in international notation

$$\boxed{\underbrace{3}_{\text{3-fold}}\underbrace{m}_{\text{Vertical mirror}} \equiv \underbrace{C_{3v}}_{\text{Name in Schönflies notation}} = \{E, C_3, C_3^2, \sigma_v, \sigma_v', \sigma_v''\}}$$

	E	C_3	C_3^2	σ_v	σ_v'	σ_v''
E	E	C_3	C_3^2	σ_v	σ_v'	σ_v''
C_3	C_3	C_3^2	E	σ_v''	σ_v	σ_v'
C_3^2	C_3^2	E	C_3	σ_v'	σ_v''	σ_v
σ_v	σ_v	σ_v'	σ_v''	E	C_3	C_3^2
σ_v'	σ_v'	σ_v''	σ_v	C_3^{-1}	E	C_3
σ_v''	σ_v''	σ_v	σ_v'	C_3	C_3^2	E

★ check
Rearrangement theorem works here too!

★ Note:
C_3 is a "subgroup" of C_{3v}.



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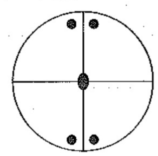
Representation of a Symmetry Group

Consider the crystallographic group C_{2v}:

- C_{2v}
- mm2
- Schönflies / international: $\{E, C_{2x_3}, \sigma_{x_1}, \sigma_{x_2}\} \equiv \{1, 2_{x_3}, m_{x_1}, m_{x_2}\}$
- $*22$ ← "orbifold" notation.
- 3D space: $\left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}$
- 4 Dimensional Space!: $\left\{ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \right\}$

- 

mm2

- 2D space: $\left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \right\}$
- 1D space:

$$\left.\begin{matrix} \{1, & -1, & 1, & -1\} \\ \{1, & -1, & -1, & 1\} \\ \{1, & 1, & 1, & 1\} \\ \{1, & 1, & -1, & -1\} \end{matrix}\right\} \text{irreducible representation } \boxed{\text{(irrep)}}$$

"Trace" Sum of the above four 1D reps: $\{4, 0, 0, 0\}$

"Trace" Sum of the first 3 1D reps: $\{3, -1, 1, 1\}$

} reducible representation. (rep)

Representation of a Symmetry Group

Consider the crystallographic group C_{2v}:

$$\left\{ \begin{pmatrix} \boxed{1} & & & \\ & \boxed{1} & & \\ & & \boxed{1} & \\ & & & \boxed{1} \end{pmatrix}, \begin{pmatrix} \boxed{-1} & & & \\ & \boxed{-1} & & \\ & & \boxed{1} & \\ & & & \boxed{1} \end{pmatrix}, \begin{pmatrix} \boxed{1} & & & \\ & \boxed{-1} & & \\ & & \boxed{1} & \\ & & & \boxed{-1} \end{pmatrix}, \begin{pmatrix} \boxed{-1} & & & \\ & \boxed{1} & & \\ & & \boxed{1} & \\ & & & \boxed{-1} \end{pmatrix} \right\}$$

Reducible representation.

- In the above example, these are the irreducible reps.

$$\{\boxed{1}, \boxed{-1}, \boxed{1}, \boxed{-1}\}$$
$$\{\boxed{1}, \boxed{-1}, \boxed{-1}, \boxed{1}\}$$
$$\{\boxed{1}, \boxed{1}, \boxed{1}, \boxed{1}\}$$
$$\{\boxed{1}, \boxed{1}, \boxed{-1}, \boxed{-1}\}$$

four irreducible representations for C_{2v}.

Character Table

- For the above example of C_{2v}, the following is called the "character table".

C_{2v}	E	C_2 ~ // to z	$\sigma_v(xz)$ ~ mirror in xz plane	$\sigma_v'(yz)$ ~ mirror in yz plane		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

Why Character Tables?

C_{2v}	E	C_2 ~ ∥ to z	$\sigma_v(xz)$ ~ mirror in xz plane	$\sigma_v'(yz)$ ~ mirror in yz plane		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

- Questions: What does this mean? Why should we care?

Some Answers:

⇒ This is the most fundamental matrix representation of C_{2v} group. (Hence "irreducible")

⇒ Any other matrix representation of C_{2v} can be built up by linearly combining A_1, A_2, B_1, B_2. Any such combination will be "reducible".

⇒ A molecule with C_{2v} Symmetry can be "perturbed", or can "vibrate", with only 4 fundamental moves. All other vibrations can be resolved into a combination of $A_1, A_2, B_1,$ & B_2 moves.

⇒ An electron wavefunction with C_{2v} Symmetry can be built with only 4 orbitals with symmetries of A_1, A_2, B_1, B_2

Examples of Character Tables

☆ Some more examples of the Character Tables:

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

$\chi\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = 2$ character.

$\chi\begin{pmatrix}-\sin 30^\circ & \cos 30^\circ\\ -\cos 30^\circ & -\sin 30^\circ\end{pmatrix}$

$\chi\begin{pmatrix}-1 & 0\\ 0 & +1\end{pmatrix}$

C_3	E	C_3	C_3^2		
A	1	1	1	$z,\ R_z$	$x^2+y^2,\ z^2$
E	$\begin{cases}1\\1\end{cases}$	$\begin{matrix}\varepsilon\\ \varepsilon^*\end{matrix}$	$\left.\begin{matrix}\varepsilon^*\\ \varepsilon\end{matrix}\right\}$	$(x,y)\ (R_x,R_y)$	$(x^2-y^2, xy)\ (yz, xz)$

$\varepsilon = \exp\left(\frac{2\pi i}{3}\right)$

S_6	E	C_3	C_3^2	i	S_6^5	S_6		
A	1	1	1	1	1	1	R_z	$x^2+y^2,\ z^2$
E_g	$\begin{cases}1\\1\end{cases}$	$\begin{matrix}\varepsilon\\ \varepsilon^*\end{matrix}$	$\begin{matrix}\varepsilon^*\\ \varepsilon\end{matrix}$	$\begin{matrix}1\\1\end{matrix}$	$\begin{matrix}\varepsilon\\ \varepsilon^*\end{matrix}$	$\left.\begin{matrix}\varepsilon^*\\ \varepsilon\end{matrix}\right\}$	(R_x,R_y)	$(x^2-y^2, x,y);\ (xz,yz)$
A_u	1	1	1	-1	-1	-1	z	
E_u	$\begin{cases}1\\1\end{cases}$	$\begin{matrix}\varepsilon\\ \varepsilon^*\end{matrix}$	$\begin{matrix}\varepsilon^*\\ \varepsilon\end{matrix}$	$\begin{matrix}-1\\-1\end{matrix}$	$\begin{matrix}-\varepsilon\\ -\varepsilon^*\end{matrix}$	$\left.\begin{matrix}-\varepsilon^*\\ -\varepsilon\end{matrix}\right\}$	(x,y)	

$\varepsilon = \exp\left(\frac{2\pi i}{3}\right)$

Why are they called Character Tables?

- Character "χ" of a matrix is the sum of its diagonal terms:

$$\chi \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = 1+1 = 2$$

$$\chi \begin{pmatrix} -\sin 30^\circ & \cos 30^\circ \\ -\cos 30^\circ & -\sin 30^\circ \end{pmatrix} = -\sin 30^\circ - \sin 30^\circ = -1 \quad \text{etc.}$$

- Character of a matrix is an invariant under Linear Orthogonal, "Similarity" transformations

proof: If E and F are conjugate matrices related by a similarity transform, then say

$$E = G^{-1} F G$$

where G is another matrix.

Then,

$$\chi(E) = \chi(G^{-1}FG) = \chi(G^{-1}GF) = \chi(F)$$

$$\Rightarrow \chi(E) = \chi(F)$$ ← Characters of conjugate matrices are equal.

The Great Orthogonality Theorem (GOT)

The great orthogonality theorem may then be stated as follows:

$$\sum_R [\Gamma_i(R)_{mn}][\Gamma_j(R)_{m'n'}]^* = \frac{h}{\sqrt{l_i l_j}} \delta_{ij}\delta_{mm'}\delta_{nn'}. \qquad (4.3\text{-}1)$$

This means that in the set of matrices constituting any one irreducible representation any set of corresponding matrix elements, one from each matrix, behaves as the components of a vector in h-dimensional space such that all these vectors are mutually orthogonal, and each is normalized so that the square of its length equals h/l_i. This interpretation of 4.3-1 will perhaps be

The Great Orthogonality Theorem (GOT)

$$\sum_R [\Gamma_i(R)_{mn}][\Gamma_j(R)_{m'n'}]^* = \frac{h}{\sqrt{l_i l_j}}\delta_{ij}\delta_{mm'}\delta_{nn'}.$$

- Pictorially, consider the following reducible representation for say a group with 4 element, R_1, R_2, R_3, R_4.

then, $\boxed{\text{example:}}$

$$\left\{ \underset{R_1}{\begin{array}{c|cccc} & 1D & 1D & 2D & \\ \hline A_1 & \Gamma_1(R_1)_{11} & & & \\ A_2 & & \Gamma_2(R_1)_{22} & & \\ E & & & \Gamma_3(R_1)_{33} & \Gamma_3(R_1)_{34} \\ & & & \Gamma_3(R_1)_{43} & \Gamma_3(R_1)_{44} \end{array}},\ \underset{R_2}{\begin{pmatrix} \Gamma_1(R_2)_{11} & & & \\ & \Gamma_2(R_2)_{22} & & \\ & & \Gamma_3(R_2)_{33} & \Gamma_3(R_2)_{34} \\ & & \Gamma_3(R_2)_{43} & \Gamma_3(R_2)_{44} \end{pmatrix}},\ \underset{R_3}{\begin{pmatrix} \Gamma_1(R_3)_{11} & & & \\ & \Gamma_2(R_3)_{22} & & \\ & & \Gamma_3(R_3)_{33} & \Gamma_3(R_3)_{34} \\ & & \Gamma_3(R_3)_{43} & \Gamma_3(R_3)_{44} \end{pmatrix}},\ \underset{R_4}{\begin{pmatrix} \Gamma_1(R_4)_{11} & & & \\ & \Gamma_2(R_4)_{22} & & \\ & & \Gamma_3(R_4)_{33} & \Gamma_3(R_4)_{34} \\ & & \Gamma_3(R_4)_{43} & \Gamma_3(R_4)_{44} \end{pmatrix}} \right\}$$

- In other words, the follow vectors in 4-dimensional space are orthogonal:

A_1 ($V_1: \{\Gamma_1(R_1)_{11}, \Gamma_1(R_2)_{11}, \Gamma_1(R_3)_{11}, \Gamma_1(R_4)_{11}\}$ ~ $(\text{length})^2 = 4$

A_2 ($V_2: \{\Gamma_2(R_1)_{22}, \Gamma_2(R_2)_{22}, \Gamma_2(R_3)_{22}, \Gamma_2(R_4)_{22}\}$ $(\text{length})^2 = 4$

E (

$V_3: \{\Gamma_3(R_1)_{33}, \Gamma_3(R_2)_{33}, \Gamma_3(R_3)_{33}, \Gamma_3(R_4)_{33}\}$ $(\text{length})^2 = 2$

$V_4: \{\Gamma_3(R_1)_{34}, \Gamma_3(R_2)_{34}, \Gamma_3(R_3)_{34}, \Gamma_3(R_4)_{34}\}$ $(\text{length})^2 = 2$

$V_5: \{\Gamma_3(R_1)_{43}, \Gamma_3(R_2)_{43}, \Gamma_3(R_3)_{43}, \Gamma_3(R_4)_{43}\}$ $(\text{length})^2 = 2$

$V_6: \{\Gamma_3(R_1)_{44}, \Gamma_3(R_2)_{44}, \Gamma_3(R_3)_{44}, \Gamma_3(R_4)_{44}\}$ $(\text{length})^2 = 2$

Five Cool Rules of Character Tables

These rules arise from the **Great Orthogonality Theorem (GOT)**

C_{2v}	E	C_2 ~ // to z	$\sigma_v(xz)$ ~ mirror in xz plane	$\sigma_v'(yz)$ ~ mirror in yz plane		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

RULE 1: $\boxed{\sum_i l_i^2 = h}$ order of the group.

$l_i \equiv$ dimension of i^{th} irrep.

e.g for C_{2v}, so 4 irreps, $i = 1, 2, 3, 4$.
each of them is 1-D, so $l_1 = l_2 = l_3 = l_4 = 1$

$h =$ order of C_{2v} = # of elements in C_{2v} = 4 = h

Check: $\sum l_i^2 = 1^2 + 1^2 + 1^2 + 1^2 = 4 = h$

$h = 4$

We can also write Rule 1 as

$$\boxed{\sum_i [\chi_i(E)]^2 = h}$$

$\chi_i(E)$ = Character of E in i^{th} irrep. $= l_i$

Five Cool Rules of Character Tables

C_{2v}	E	C_2 (// to z)	$\sigma_v(xz)$ (mirror in xz plane)	$\sigma_v'(yz)$ (mirror in yz plane)		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

RULE 2:

$$\boxed{\sum_R [\chi_i(R)]^2 = h}$$

e.g. C_{2v}

For

A_1: $1^2 + 1^2 + 1^2 + 1^2 = 4$

A_2: $1^2 + 1^2 + (-1)^2 + (-1)^2 = 4$

B_1: $1^2 + (-1)^2 + 1^2 + (-1)^2 = 4$

B_2: $1^2 + (-1)^2 + (-1)^2 + 1^2 = 4$

In C_{3v},

A_1: $1^2 + 2\times(1)^2 + 3\times(+1)^2 = 6$

A_2: $1^2 + 2\times(1)^2 + 3\times(-1)^2 = 6$

E: $\cancel{1}\times 2^2 + 2\times(-1)^2 = 6$

Five Cool Rules of Character Tables

C_{2v}	E	C_2 (// to z)	$\sigma_v(xz)$ (mirror in xz plane)	$\sigma_v'(yz)$ (mirror in yz plane)		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

Rule 3

$$\boxed{\sum_R \chi_i(R)\,\chi_j(R) = 0} \quad \text{when} \quad i \neq j$$

e.g C_{2v}, Consider $A_1 = i$ & $A_2 = j$;

$$1(1) + 1(1) + 1(-1) + 1(-1) = 0$$

In C_{3v} $A_1 = i$ & $A_2 = j$,

$$1(1) + 2 \times 1(1) + 3 \times 1(-1) = 0$$

and so on for other pairs of A_1, A_2; B_1, B_2

Five Cool Rules of Character Tables

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	-1	R_z	
E	2	-1	0	$(x,y)\ (R_x, R_y)$	$(x^2-y^2, xy)\ (xz, yz)$
	$\chi\begin{pmatrix}1&0\\0&1\end{pmatrix}=2$	$\chi\begin{pmatrix}-\sin 30^\circ & \cos 30^\circ\\ -\cos 30^\circ & -\sin 30^\circ\end{pmatrix}$	$\chi\begin{pmatrix}-1&0\\0&+1\end{pmatrix}$		

character.

Rule 4

$$\boxed{\chi_i(R_1) = \chi_i(R_2)}$$

if R_1, R_2 are in the same class.

e.g. C_3 & C_3^{-1} in C_{3v} group are conjugates, (i.e they are related by Similarity Transform). Hence

$$\boxed{\chi_i(C_3) = \chi_i(C_3^{-1})} \quad \text{in } C_{3v}$$

Similarly the three mirrors σ_v, σ_v', σ_v'' are conjugates

$$\chi_i(\sigma_v) = \chi_i(\sigma_v') = \chi(\sigma_v'')$$

Proof: we already showed that χ in invariant with similarity transform.

Five Cool Rules of Character Tables

C_{2v}	E	C_2 (// to z)	$\sigma_v(xz)$ (mirror in xz plane)	$\sigma_v'(yz)$ (mirror in yz plane)		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

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

$\chi\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = 2$ character

$\chi\begin{pmatrix}-\sin 30^\circ & \cos 30^\circ\\ -\cos 30^\circ & -\sin 30^\circ\end{pmatrix}$

$\chi\begin{pmatrix}-1 & 0\\ 0 & +1\end{pmatrix}$

Rule 5

$\boxed{\#\text{ of irreps} = \#\text{ of classes}}$

In C_{2v} : $4 = 4$

In C_{3v} : $3 = 3$

Constructing a Character Table for C_{3v} using the Five Cool Rules

$\boxed{\text{Example for } C_{3v}}$

- Let us construct the Character Table for C_{3v}.

$$C_{3v} = \{E,\ 2C_3,\ 3\sigma_v\}$$

Six elements, so $h = 6$

3 classes, so $i = \#\text{ irreps} = 3$

- From rule 1, we know that

$$l_1^2 + l_2^2 + l_3^2 = h = 6$$

The only way this is possible is if

$$1^2 + 1^2 + 2^2 = 6$$

$$\Rightarrow \quad l_1 = 1, \quad l_2 = 1, \quad l_3 = 2$$

- Every Character Table must have an A_1 with all 1's.

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2			
E			

Constructing a Character Table for C_{3v} using the Five Cool Rules

- Using Rule 3,

$$\chi_{A_1}(E)\,\chi_{A_2}(E) + 2\times\chi_{A_1}(C_3)\,\chi_{A_2}(C_3) + 3\,\chi_{A_1}(\sigma_v)\,\chi_{A_2}(\sigma_v) = 0$$

$$\Rightarrow \quad \chi_{A_2}(E) + 2\,\chi_{A_2}(C_3) + 3\,\chi_{A_2}(\sigma_v) = 0$$

Clearly,

$$1 + 2\times 1 + 3\times(-1) = 0$$

$\Rightarrow$ so

$$\chi_{A_2}(E) = 1 \qquad \chi_{A_2}(C_3) = 1 \qquad \chi_{A_2}(\sigma_v) = -1$$

Note: $\boxed{\chi(E) \text{ is always positive!}}$ (=1 for 1D, 2 for 2D, 3 for 3D)

$\Rightarrow$

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	−1
E	2		

- For the "E" irrep: Rule 1 gives

$$2^2 + 2\times\chi_E(C_3)^2 + 3\times\chi_E(\sigma_v)^2 = 6$$

$$\Rightarrow \quad 2\,\chi_E(C_3)^2 + 3\,\chi_E(\sigma_v)^2 = 2$$

$$\Rightarrow \quad \chi_E^2(C_3) = 1 \quad \text{or} \quad \boxed{\chi_E(C_3) = \pm 1}$$

Which is it? See next.

P.14

- From rule 3:

$\cancel{\chi_E(A_2)\,\chi_E(E) + 2\,\chi_{C_3}}$

$$\chi_{A_2}(E)\,\chi_E(E) + 2\times\chi_{A_2}(C_3)\,\chi_E(C_3) + 3\,\chi_{A_2}(\sigma_v)\,\chi_E(\sigma_v) = 0$$

$$\Rightarrow \quad 1\times 2 + 2\times 1\times\chi_E(C_3) + 3\,(-1)\,\chi_E(\sigma_v) = 0$$

$$\Rightarrow \quad \chi_E(C_3) = -1 \quad \& \quad \chi_E(\sigma_v) = 0$$

Constructing a Character Table for C_{3v} using the Five Cool Rules

Hence the Character Table is Complete :

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2+y^2,\ z^2$
A_2	1	1	−1	R_z	
E	2	−1	0 $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$(x,y)\ (R_x, R_y)$	$(x^2-y^2, xy)\ (xz, yz)$
I	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	II $\begin{pmatrix} \cos 120° & -\sin 120° \\ \sin 120° & \cos 120° \end{pmatrix}$		III	IV

Reading a Character Table

Reading a Character Table :

- Column 1 : Labels for the irreps. (R.S. Mulliken Symbols)

All 1-D irreps ≡ A or B
2-D irreps ≡ E (but we will label as $\mathcal{E}$ to avoid confusion with identity E)
3-D irreps ≡ T (or F sometimes)

If $\boxed{\chi(C_n) = 1}$, then A
if $\boxed{\chi(C_n) = -1}$, then B
principal rotation axis.

A_1, B_1 means $\boxed{\chi(C_2) = +1}$ where $C_2 \perp C_n$ (the principle rotation axis).

A_2, B_2 means $\boxed{\chi(C_2) = -1}$ where $C_2 \perp C_n$

If a $C_2 \perp C_n$ is absent, then $\chi(\sigma_v)$ is considered

Prime and Double prime :

A', B' etc : $\chi(\sigma_h) = +1$
A'', B'' etc : $\chi(\sigma_h) = -1$

e.g

C_s	E	σ_h		
A'	1	1	x, y, R_z	x^2, y^2, z^2, xy
A''	1	-1	z, R_x, R_y	yz, xz

Inversion : A_g, B_g, E_g etc $\boxed{\chi(i) = +1}$
A_u, B_u, E_u etc $\boxed{\chi(i) = -1}$

Constructing a Character Table for D_4 using the Five Cool Rules

- $D_4 = \{E,\ C_4,\ C_4^2 = C_2,\ C_4^{-1} = C_4^3,\ C_{2,x},\ C_{2,y},\ C'_{2,xy},\ C'_{2,x\bar{y}}\}$

- Gather into classes : $\{\underbrace{(E)}_{\text{classes}}, (2C_4), (C_{2z} = C_4^2), (\underbrace{2C_2}_{C_{2x},\, C_{2y}}), (\underbrace{2C_2'}_{C_{2,xy},\, C_{2,x\bar{y}}})\}$

  5 (classes) = 5 irreps.

-

D_4	E	$2C_4$	$C_{2z} = C_4^2$	$2C_2$	$2C_2'$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
	1				
	1				
E	2				

↓ see below.

5 irreps

This irrep is always there

See below for these

- $l_1^2 + l_2^2 + l_3^2 + l_4^2 + l_5^2 = 8$ ~ order of the group.

  $\Rightarrow \underbrace{l_1 = l_2 = l_3 = l_4 = 1}_{\text{4 1-Dimensional irreps}} \quad \underbrace{l_5 = 2}_{\text{1 2-D irrep.}}$

Constructing a Character Table for D_4 using the Five Cool Rules

- $$\sum_R \chi^2(R) = h$$

e.g. A_1: $1\times1^2 + 2\times1^2 + 1\times1^2 + 2\times1^2 + 2\times1^2 = 8$

Another Solution is Clearly:

$$1\times1^2 + 2\times1^2 + 1\times1^2 + 2\times(-1)^2 + 2\times(-1)^2 = 8$$

and... it satisfies orthogonality condition:

$$\sum_R \underbrace{\chi_1(R)\,\chi_2(R)}_{\text{different irreps 1 \& 2.}} = 0$$

$$1\times1 + 2\times1\times1 + 1\times1 + 2\times1\times-1 + 2\times1\times-1 = 0$$

LP.1

- Since $\chi(C_4) = +1$ & $\chi(C_2 \perp C_4) = -1$, we label this as $\boxed{A_2 \equiv 1 \quad 1 \quad 1 \quad -1 \quad -1}$

- Clearly, you can permute the "−" signs among the three classes $2C_4$, $2C_2$ & $2C_2'$ and still get the same results as above. So we get two more:

	E	$2C_4$	$C_4^2=C_2$	$2C_2$	$2C_2'$
B_1	1	−1	1	1	−1
B_2	1	−1	1	−1	1
E	2	0	−2	0	0

Since $\chi(C_4)=-1$ and $\chi(C_2)=1$ (B_1)

Since $\chi(C_4)=-1$ and $\chi(C_2)=-1$ (B_2)

See below.

Constructing a Character Table for D_4 using the Five Cool Rules

- That leaves the 2-D irrep $\mathcal{E}$.

$$\mathcal{E} \cdot A_1 = 0$$

$$\Rightarrow 1 \times 2 \times 1 + 2 \times (a) \times 1 + 1 \times (b) \times 1 + 2 \times (c) \times 1 + 2 \times (d) \times 1 = 0$$

$$\mathcal{E} \cdot A_2 = 0$$

$$\Rightarrow 1 \times 2 \times 1 + 2 \times (a) \times 1 + 1 \times (b) \times 1 + 2 \times (c) \times (-1) + 2 \times (d) \times (-1) = 0$$

The only way both the above conditions can be satisfied is if

$$(a \;\; b \;\; c \;\; d) = (0 \;\; -2 \;\; 0 \;\; 0)$$

- This completes the character Table, as shown below.

D_4	E	$2C_4$	$C_{2z} = C_4^2$	$2C_2$	$2C_2'$		
A_1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	-1	-1	z, R_z	
B_1	1	-1	1	1	-1		x^2-y^2
B_2	1	-1	1	-1	1		xy
$\mathcal{E}$	2	0	-2	0	0	(x,y), (R_x,R_y)	(xz, yz)
	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$		

Character Table for Cyclic Groups

- A "cyclic group" is an abelian group where all elements commute, and each element is in its own class.

- Pick any rotation axis C_n. Then,

  $$\mathcal{C}_n \equiv \{C_n^1, C_n^2, C_n^3, C_n^4, \ldots, C_n^n = E\}$$ ~ forms a group. (cyclic)

  ⇒ elements commute: e.g. $C_n^2 \cdot C_n^3 = C_n^3 \cdot C_n^2 = C_n^5$

  ⇒ Each element is in its own class: e.g. $(C_n^p)^{-1} C_n^2 (C_n^p)$ = Conjugate of C_n^2

  $\boxed{\text{i.e. element} \equiv \text{its own conjugate}}$ $= (C_n^p)^{-1} (C_n^p) C_n^2 = C_n^2$

- What is the character Table for $\mathcal{C}_n$?

  ⇒ e.g. pick $\mathcal{C}_3 \equiv \{C_3, C_3^2, C_3^3 = E\}$

  Three classes, so three irreps.

$\mathcal{C}_3$	$C_3^3=E$	C_3	C_3^2
A_1	1	1	1
Γ_1	1	a?	b?
Γ_2	1	c?	d?

Temporary names for irreps. (Γ_1, Γ_2)

Character Table for Cyclic Group, C_3

- What is the character Table for $\mathcal{C}_n$?

⇒ e.g. pick $\mathcal{C}_3 = \{C_3, C_3^2, C_3^3 = E\}$

Three classes, so three irreps.

$\mathcal{C}_3$	$C_3^3 = E$	C_3	C_3^2
A_1	1	1	1
Γ_1'	1	a?	b?
Γ_2'	1	c?	d?

Temporary names for irreps.

⇒ $\sum_i l_i^2 = h = 3$ order of the group.

dimension of irrep "i".

$$1^2 + 1^2 + 1^2 = 3$$

⇒ $l_1 = l_2 = l_3 = 1$ three 1-D irreps.

⇒ Now $\sum_R \chi_i^2(R) = h = 3$

for A_1 : $1^2 + 1^2 + 1^2 = 3$

for Γ_1' : $1^2 + a^2 + b^2 = 3$

for Γ_2' : $1^2 + c^2 + d^2 = 3$

what are a, b, c, d? clearly there are no more real integers as solutions.

⇒ a, b, c, d must be complex numbers.

Character Table for Cyclic Group, C_3

You can check that $a = e^{i\frac{2\pi}{3}}$ and $b = e^{-i\frac{2\pi}{3}}$ works:

$$1^2 + \underbrace{e^{i\frac{2\pi}{3}} \cdot e^{-i\frac{2\pi}{3}}}_{a \cdot a^* = |a|^2} + \underbrace{e^{-i\frac{2\pi}{3}}\, e^{i\frac{2\pi}{3}}}_{b \cdot b^* = |b|^2} = 3$$

$a^* \equiv$ complex conjugate of a

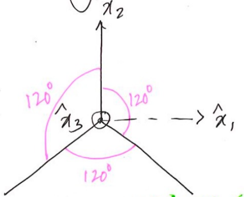
The $\boxed{\text{complete character table}}$ looks like:

C_3	$C_3^3 = E$	C_3^1	$C_3^2 = C_3^{-1}$		
A_1	1	1	1	z, R_z	x^2+y^2, z^2
Γ_1	1	$e^{i\frac{2\pi}{3}}$	$e^{-i\frac{2\pi}{3}}$	(x,y) (R_x, R_y)	$(x^2-y^2, xy), (yz, xz)$
Γ_2	1	$e^{-i\frac{2\pi}{3}}$	$e^{i\frac{2\pi}{3}}$		

Together, they are called E, a 2-D irrep.

Complex irreps

- Why are T_1 and T_2 together called $\mathcal{E}$, a 2-D irrep?



$$C_3 = \begin{pmatrix} \cos 120^\circ & \sin 120^\circ & 0 \\ -\sin 120^\circ & \cos 120^\circ & 0 \\ 0 & 0 & \boxed{1} \end{pmatrix}$$

2D irrep, $\mathcal{E}$

1D irrep

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \boxed{1} \end{pmatrix}$$

2D irrep (see C_3 & C_3^{-1})

1D

$$C_3^{-1} = \begin{pmatrix} \cos 120^\circ & -\sin 120^\circ & 0 \\ \sin 120^\circ & \cos 120^\circ & 0 \\ 0 & 0 & \boxed{1} \end{pmatrix}$$

2D irrep

1D

⇒ Consider the 2D irrep:

	E	C_3	C_3^{-1}
$\mathcal{E}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \cos\frac{2\pi}{3} & \sin\frac{2\pi}{3} \\ -\sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} \end{pmatrix}$	$\begin{pmatrix} \cos\frac{2\pi}{3} & -\sin\frac{2\pi}{3} \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} \end{pmatrix}$
$\mathcal{E}$	$\chi(\mathcal{E}) = 2$	$\chi(\mathcal{E}) = 2\cos\frac{2\pi}{3}$	$\chi(\mathcal{E}) = 2\cos\frac{2\pi}{3}$

⇒ Now compare with the Table below:

	E	C_3	C_3^{-1}
$\mathcal{E}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \epsilon & 0 \\ 0 & \epsilon^* \end{pmatrix}$	$\begin{pmatrix} \epsilon^* & 0 \\ 0 & \epsilon \end{pmatrix}$

$\epsilon = \exp\left(i\frac{2\pi}{3}\right)$

$\epsilon^* = \exp\left(-i\frac{2\pi}{3}\right)$

$\mathcal{E}$	$\chi(\mathcal{E}) = 2$	$\chi(\mathcal{E}) = \epsilon + \epsilon^* = 2\cos\frac{2\pi}{3}$	$\chi(\mathcal{E}) = \epsilon^* + \epsilon = 2\cos\frac{2\pi}{3}$

- The characters are the same for the complex irreps and the real version of the irreps.

Character Table for a General C_n

Representation for a general C_n

C_n^i	C_n	C_n^2	C_n^3	C_n^4	$\cdots$	$C_n^n = E$
Γ_1	ϵ	ϵ^2	ϵ^3	ϵ^4	$\cdots$	$\epsilon^n = 1$
Γ_2	ϵ^2	ϵ^4	ϵ^6	ϵ^8	$\cdots$	$\epsilon^{2n} = 1$
Γ_3	ϵ^3	ϵ^6	ϵ^9	ϵ^{12}	$\cdots\ \epsilon^{3n-3}$	$\epsilon^{3n} = 1$
Γ_4	ϵ^4	ϵ^8	ϵ^{12}	ϵ^{16}	$\cdots\ \epsilon^{4n-8}\ \epsilon^{4n-4}$	$\epsilon^{4n} = 1$
$\vdots$						
Γ_n	$\epsilon^n = 1$	$\epsilon^{2n} = 1$	$\epsilon^{3n} = 1$	$\epsilon^{4n} = 1$	$\cdots$	$\epsilon^{n^2} = 1$

where $\boxed{\epsilon = \exp\left(i\,\frac{2\pi}{n}\right)}$