C_{3v}

Definition

C_{3v} is the symmetry group of an equilateral triangle.
(The upper & lower faces of the triangle are assumed to be different)

With reference to the figure,

```
        3              (o is center of gravity )
       / \
      / o \
     / ___ \
    1       2
```

the symmetry operations are

σ_i: reflection about the vertical plane that contains the line thru *oi*. ($i = 1, 2, 3$).

C_3 [C_3^2]: Rotation by $\frac{2\pi}{3}$ [$\frac{4\pi}{3}$] about the vertical axis that passes thru *o*.

Multiplication Table

C_{3v}	e	σ_1	σ_2	σ_3	C_3	C_3^2
e	e	σ_1	σ_2	σ_3	C_3	C_3^2
σ_1	σ_1	e	C_3	C_3^2	σ_2	σ_3
σ_2	σ_2	C_3^2	e	C_3	σ_3	σ_1
σ_3	σ_3	C_3	C_3^2	e	σ_1	σ_2
C_3	C_3	σ_3	σ_1	σ_2	C_3^2	e
C_3^2	C_3^2	σ_2	σ_3	σ_1	e	C_3

Classes

e, $\{\sigma_1, \sigma_2, \sigma_3\}$, $\{C_3, C_3^2\}$

Subgroups

All subgroups are abelian;
$H_1 = \{e, \sigma_1\}$, $H_2 = \{e, \sigma_2\}$, $H_3 = \{e, \sigma_3\}$, $H_4 = \{e, C_3, C_3^2\}$

Furthermore, H_4 is an invariant subgroup.
Thus, C_{3v} is not simple.
Since H_4 is abelian, C_{3v} is not semi-simple.

Cosets & Factor Groups

$H_1 = \{ e, \sigma_1 \}$

The left cosets are

$$\sigma_2 H_1 = \left\{ \sigma_2, C_3^2 \right\} = C_3^2 H_1$$

$$\sigma_3 H_1 = \{ \sigma_3, C_3 \} = C_3 H_1$$

The right cosets are

$$H_2 \sigma_2 = \{ \sigma_2, C_3 \} = H_2 C_3$$

$$H_2 \sigma_3 = \left\{ \sigma_3, C_3^2 \right\} = H_2 C_3^2$$

$H_4 = \left\{ e, C_3, C_3^2 \right\}$

The left cosets are

$$\sigma_1 H_4 = \{ \sigma_1, \sigma_2, \sigma_3 \} = \sigma_2 H_4 = \sigma_3 H_4$$

The right cosets are

$$H_4 \sigma_1 = \{ \sigma_1, \sigma_2, \sigma_3 \} = H_4 \sigma_2 = H_4 \sigma_3$$

Hence, the left & right cosets are equal, as is expected since H_4 is an invariant subgroup.

We thus expect a factor group

$$C_{3v}/H_4 = C_{3v}/C_3 \qquad [\ C_3 \text{ is the cyclic group } \left\{ e, C_3, C_3^2 \right\}\ ]$$

To show that C_{3v}/H_4 is indeed a group, we calculate its multiplication table:

$$H_4 \cdot H_4 = \left\{ e, C_3, C_3^2 \right\} \cdot \left\{ e, C_3, C_3^2 \right\} = H_4$$

$$H_4 \cdot \sigma_1 H_4 = \left\{ e, C_3, C_3^2 \right\} \cdot \{ \sigma_1, \sigma_2, \sigma_3 \} = \{ \sigma_1, \sigma_2, \sigma_3 \} = \sigma_1 H_4$$

$$\sigma_1 H_4 \cdot H_4 = \{ \sigma_1, \sigma_2, \sigma_3 \} \cdot \left\{ e, C_3, C_3^2 \right\} = \{ \sigma_1, \sigma_2, \sigma_3 \} = \sigma_1 H_4$$

$$\sigma_1 H_4 \cdot \sigma_1 H_4 = \{ \sigma_1, \sigma_2, \sigma_3 \} \cdot \{ \sigma_1, \sigma_2, \sigma_3 \} = \left\{ e, C_3, C_3^2 \right\} = H_4$$

ie.

C_{3v}/H_4	H_4	$\sigma_1 H_4$
H_4	H_4	$\sigma_1 H$
$\sigma_1 H$	$\sigma_1 H$	H_4

This is the same as the multiplication table for the cyclic group $C_2 = \{e, C_2\}$.
Therefore

$$C_{3v}/C_3 = C_2$$

Note that C_2 is a subgroup of C_{3v}. [Actually, there're 3 of them: H_1, H_2 & H_3]
However, C_2 is not an invariant subgroup so that

$$C_3 \otimes C_2 \neq C_{3v}$$

In fact,

$$C_3 \otimes C_2 = C_{3h} = \left\{ e, C_3, C_3^2, \sigma_h, S_3, S_3^2 \right\}$$

where

σ_h = reflection across a plane perpendicular to the C_3 rotation axis.

$S_3 = \sigma_h C_3$ and $S_3^2 = \sigma_h C_3^2$ are "screw" rotations.

Note that C_{3h} is abelian & isomorphic to C_6.

IRs

To satisfy

$$\sum_{\mu=1}^{n_c} n_\mu{}^2 = n_G$$

for $n_G = 6,\ n_c = 3,$

we can only have

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

Hence, there're 3 IRs with dimensions

$$n_\mu = 1,\ 1,\ 2$$

1-Dim IRs, D^1 & D^2

The two 1-D IRs are easily seen to be

C_{3v}	e	σ_1	σ_2	σ_3	C_3	$C_3{}^2$
D^1	1	1	1	1	1	1
D^2	1	−1	−1	−1	1	1

The corresponding character table is

C_{3v}	e	$3\,\sigma$	$2\,C_3$
χ^1	1	1	1
χ^2	1	−1	1

2-D Unitary IR, D^3

A 2-D unitary IR can be obtained for $V = E_2$ using orthonormal basis $\{\hat{e}_1,\ \hat{e}_2\}$ as shown in figure:

3

$\hat{e}_2$ ↑

$o \longrightarrow \hat{e}_1$

1 2

where o is center of gravity of the equilateral triangle 123.

It is easily verified that

$$D^3(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$D^3(\sigma_1) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \qquad D^3(\sigma_2) = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \qquad D^3(\sigma_3) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$D^3(C_3) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \qquad D^3\left(C_3{}^2\right) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

For example,

$$U(\sigma_1)\,\hat{e}_1 = \hat{e}_1\ D^3(\sigma_1)^1{}_1 + \hat{e}_2\ D^3(\sigma_1)^2{}_1$$
$$= \frac{1}{2}\,\hat{e}_1 + \frac{\sqrt{3}}{2}\,\hat{e}_2$$
$$U(\sigma_1)\,\hat{e}_2 = \hat{e}_1\ D^3(\sigma_1)^1{}_2 + \hat{e}_2\ D^3(\sigma_1)^2{}_2$$
$$= \frac{\sqrt{3}}{2}\,\hat{e}_1 - \frac{1}{2}\,\hat{e}_2$$

We can construct a representation table for C_{3v}:

C_{3v}	e	σ_1	σ_2	σ_3	C_3	C_3^2
D^1	1	1	1	1	1	1
D^2	1	-1	-1	-1	1	1
$[D^3]^1{}_1$	1	$\frac{1}{2}$	$\frac{1}{2}$	-1	$-\frac{1}{2}$	$-\frac{1}{2}$
$[D^3]^1{}_2$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$
$[D^3]^2{}_1$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$
$[D^3]^2{}_2$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$

where D^1 & D^2 are 1-Dim IRs.

The corresponding character table is

C_{3v}	e	$3\,\sigma$	$2\,C_3$
χ^1	1	1	1
χ^2	1	-1	1
χ^3	2	0	-1

To check the orthogonality & completeness theorems, we convert the table to

C_{3v}	e	σ_1	σ_2	σ_3	C_3	C_3^2
$D^{-1}{}_1$	1	1	1	1	1	1
$D^{-1}{}_2$	1	-1	-1	-1	1	1
$[D^{-1}{}_3]^1{}_1$	1	$\frac{1}{2}$	$\frac{1}{2}$	-1	$-\frac{1}{2}$	$-\frac{1}{2}$
$[D^{-1}{}_3]^1{}_2$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$
$[D^{-1}{}_3]^2{}_1$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$
$[D^{-1}{}_3]^2{}_2$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$

Collecting the pairs of dual vectors into adjacent rows, we have

C_{3v}	e	σ_1	σ_2	σ_3	C_3	$C_3{}^2$
D^1	1	1	1	1	1	1
$D^{-1}{}_1$	1	1	1	1	1	1
D^2	1	-1	-1	-1	1	1
$D^{-1}{}_2$	1	-1	-1	-1	1	1
$[D^3]^1{}_1$	1	$\frac{1}{2}$	$\frac{1}{2}$	-1	$-\frac{1}{2}$	$-\frac{1}{2}$
$[D^{-1}{}_3]^1{}_1$	1	$\frac{1}{2}$	$\frac{1}{2}$	-1	$-\frac{1}{2}$	$-\frac{1}{2}$
$[D^3]^1{}_2$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$
$[D^{-1}{}_3]^2{}_1$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	$-\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2}$
$[D^3]^2{}_1$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$
$[D^{-1}{}_3]^1{}_2$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$	0	$\frac{\sqrt{3}}{2}$	$-\frac{\sqrt{3}}{2}$
$[D^3]^2{}_2$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$
$[D^{-1}{}_3]^2{}_2$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$

Note that each row vector is the same as its dual.
This happens when the rep matrices are orthogonal (the basis is orthonormal).

For example, the 4th row gives

$$\sum_g D_3{}^{-1}(g)^2{}_1\, D^3(g)^1{}_2$$
$$= 0\cdot 0 + \frac{\sqrt{3}}{2}\cdot\frac{\sqrt{3}}{2} + \left(-\frac{\sqrt{3}}{2}\right)\cdot\left(-\frac{\sqrt{3}}{2}\right) + 0\cdot 0 + \left(-\frac{\sqrt{3}}{2}\right)\cdot\left(-\frac{\sqrt{3}}{2}\right) + \frac{\sqrt{3}}{2}\cdot\frac{\sqrt{3}}{2}$$
$$= 3$$
$$= \frac{n_G}{n_\mu} = \frac{6}{2} = 3$$

Similarly, the 2nd column gives

$$\frac{n_\mu}{n_G} D^\mu(\sigma_1)^l{}_k\, D_\mu{}^{-1}(\sigma_1)^k{}_l$$
$$= \frac{1}{6}\left\{ 1\cdot 1\cdot 1 + 1\cdot(-1)\cdot(-1) + 2\cdot\left[\frac{1}{2}\cdot\frac{1}{2} + \frac{\sqrt{3}}{2}\cdot\frac{\sqrt{3}}{2} + \frac{\sqrt{3}}{2}\cdot\frac{\sqrt{3}}{2} + \left(-\frac{1}{2}\right)\cdot\left(-\frac{1}{2}\right)\right]\right\}$$
$$= 1$$

- **2-D non-unitary IR, D^4**

A 2-D IR that is not unitary can be obtained using non-orthogonal basis $\{\hat{u}_1, \hat{u}_2\}$ as shown in figure:

3
$\hat{u}_3$ ↑
o
$\hat{u}_1$ ↙ ↘ $\hat{u}_2$
1 2

[u_i is the vector going from o to vertex i.]

Using

$$\hat{u}_3 = -\left(\hat{u}_1 + \hat{u}_2 \right)$$

it is easily verified that

$$D^4\,(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$D^4(\sigma_1) = \begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix} \qquad D^4(\sigma_2) = \begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix} \qquad D^4(\sigma_3) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$D^4(C_3) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} \qquad D^4\left(C_3{}^2\right) = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$$

The rep tables are:

$C_{3\,v}$	e	$\boldsymbol{\sigma}_1$	$\boldsymbol{\sigma}_2$	$\boldsymbol{\sigma}_3$	C_3	$C_3{}^2$
D^1	1	1	1	1	1	1
D^2	1	−1	−1	−1	1	1
$\left[D^4\right]^1{}_1$	1	1	−1	0	0	−1
$\left[D^4\right]^1{}_2$	0	−1	0	1	−1	1
$\left[D^4\right]^2{}_1$	0	0	−1	1	1	−1
$\left[D^4\right]^2{}_2$	1	−1	1	0	−1	0

$C_{3\,v}$	e	$\boldsymbol{\sigma}_1$	$\boldsymbol{\sigma}_2$	$\boldsymbol{\sigma}_3$	C_3	$C_3{}^2$
$D^{-1}{}_1$	1	1	1	1	1	1
$D^{-1}{}_2$	1	−1	−1	−1	1	1
$\left[D^{-1}{}_4\right]^1{}_1$	1	1	−1	0	−1	0
$\left[D^{-1}{}_4\right]^2{}_1$	0	0	−1	1	−1	1
$\left[D^{-1}{}_4\right]^1{}_2$	0	−1	0	1	1	−1
$\left[D^{-1}{}_4\right]^2{}_2$	1	−1	1	0	0	−1

$C_{3\,v}$	e	$\boldsymbol{\sigma}_1$	$\boldsymbol{\sigma}_2$	$\boldsymbol{\sigma}_3$	C_3	$C_3{}^2$
D^1	1	1	1	1	1	1
$D^{-1}{}_1$	1	1	1	1	1	1
D^2	1	−1	−1	−1	1	1
$D^{-1}{}_2$	1	−1	−1	−1	1	1
$\left[D^4\right]^1{}_1$	1	1	−1	0	0	−1
$\left[D^{-1}{}_4\right]^1{}_1$	1	1	−1	0	−1	0
$\left[D^4\right]^1{}_2$	0	−1	0	1	−1	1
$\left[D^{-1}{}_4\right]^2{}_1$	0	0	−1	1	−1	1
$\left[D^4\right]^2{}_1$	0	0	−1	1	1	−1
$\left[D^{-1}{}_4\right]^1{}_2$	0	−1	0	1	1	−1
$\left[D^4\right]^2{}_2$	1	−1	1	0	−1	0
$\left[D^{-1}{}_4\right]^2{}_2$	1	−1	1	0	0	−1

The corresponding character table is

C_{3v}	e	3σ	$2C_3$
χ^4	2	0	−1

which is the same as χ^3, as expected.

Check out the orthogonality & completeness theorems yourself.

■ Transformation

Consider 2 sets of bases $\{e_i\}$ & $\{e_i'\}$ of V.

Thus

$$x = e_i x^i = e_i' x'^i \qquad \forall\, x \in V$$

Let these bases be related by the transformation S:

$$e_i' = e_j S^j{}_i$$

then

$$x = e_i' x'^i = e_j S^j{}_i x'^i = e_i x^i$$

ie.,

$$x^i = S^i{}_j x'^j$$

or, in matrix form,

$$\boldsymbol{x} = S\,\boldsymbol{x}'$$

where

$$\boldsymbol{x} = \begin{pmatrix} x^1 \\ \vdots \\ x^i \\ \vdots \end{pmatrix} = \begin{pmatrix} \\ S^i{}_j \\ \\ \end{pmatrix} \begin{pmatrix} x'^1 \\ \vdots \\ x'^j \\ \vdots \end{pmatrix} = S\,\boldsymbol{x}'$$

or

$$\boldsymbol{x}' = S^{-1}\,\boldsymbol{x}$$

Next, an operator U on V is defined by its action on the basis:

$$U e_i = e_j D^j{}_i$$

and

$$U e_i' = e_j' D'^j{}_i$$

Thus

$$\begin{aligned} U x &= U e_i x^i \\ &= e_j D^j{}_i x^i \\ &= e_i y^i \end{aligned}$$

where

$$y^i = D^i{}_j x^j$$

or

$$\boldsymbol{y} = D\,\boldsymbol{x}$$

Similarly

$$U\,x = U\,e_i'\,x'^i$$
$$= \; e_j'\,D'^j{}_i\,x'^i$$
$$= \; e_i'\,y'^i$$

where

$$y'^i = D'^i{}_j\,x'^j$$

or

$$\boldsymbol{y}' = D'\,\boldsymbol{x}'$$

Thus

$$\boldsymbol{y} = D\,\boldsymbol{x}$$
$$= \; D\,S\,\boldsymbol{x}'$$
$$= \; S\,\boldsymbol{y}'$$

or

$$\boldsymbol{y}' = S^{-1}\,D\,S\,\boldsymbol{x}'$$
$$\equiv \; D'\,\boldsymbol{x}'$$

so that

$$D' = S^{-1}\,D\,S$$

where

$$e_i' = e_j\,S^j{}_i$$
$$\boldsymbol{x}' = S^{-1}\,\boldsymbol{x}$$

An alternative form is

$$\boldsymbol{x} = S\,\boldsymbol{x}'$$
$$e_i = e_j'\left(S^{-1}\right)^j{}_i$$
$$D = S\,D'\,S^{-1}$$

where

$$U\,e_i = e_j\,D^j{}_i$$
$$U\,e_i' = e_j'\,D'^j{}_i$$

- **$D^4 \sim D^3$**

Since there can only be 3 inequivalent IRs, D^3 & D^4 must be equivalent, ie.,

$$D^4(g) = S\,D^3(g)\,S^{-1} \qquad \forall\, g \in G$$

where

$$\hat{u}_i = \hat{e}_j\left(S^{-1}\right)^j{}_i \qquad \hat{e}_i = \hat{u}_j\,S^j{}_i$$

[see section "Transformation"]

Note that the orthogonality theorem cannot be applied to equivalent IRs of dim greater than 1, eg., $D^3(g)^i{}_j$ & $D^4(g)^k{}_l$ since the indices $i,\ j$ refer to a basis different from that for $k,\ l$.

Setting the unit length as the distance $o\,i$, we have

$$\hat{u}_1 = -\frac{\sqrt{3}}{2}\,\hat{e}_1 - \frac{1}{2}\,\hat{e}_2 \qquad \hat{e}_1 = -\frac{1}{\sqrt{3}}\,\hat{u}_1 + \frac{1}{\sqrt{3}}\,\hat{u}_2$$

$$\hat{u}_2 = \frac{\sqrt{3}}{2}\,\hat{e}_1 - \frac{1}{2}\,\hat{e}_2 \qquad \hat{e}_2 = -\hat{u}_1 - \hat{u}_2$$

so that

$$S^{-1} = \begin{pmatrix} -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\ -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \qquad S = \begin{pmatrix} -\frac{1}{\sqrt{3}} & -1 \\ \frac{1}{\sqrt{3}} & -1 \end{pmatrix}$$

Thus, for example,

$$\begin{aligned} S\,D^3(\sigma_1)\,S^{-1} &= \begin{pmatrix} -\frac{1}{\sqrt{3}} & -1 \\ \frac{1}{\sqrt{3}} & -1 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\ -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \\ &= \begin{pmatrix} -\frac{1}{\sqrt{3}} & -1 \\ \frac{1}{\sqrt{3}} & -1 \end{pmatrix} \begin{pmatrix} -\frac{\sqrt{3}}{2} & 0 \\ -\frac{1}{2} & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix} \\ &= D^4(\sigma_1) \end{aligned}$$

▪ D^R

To get D^R, we 1st re-write the multiplication table as

C_{3v}	$e^{-1} = e$	$\boldsymbol{\sigma}_1{}^{-1} = \boldsymbol{\sigma}_1$	$\boldsymbol{\sigma}_2{}^{-1} = \boldsymbol{\sigma}_2$	$\boldsymbol{\sigma}_3{}^{-1} = \boldsymbol{\sigma}_3$	$C_3{}^{-1} = C_3{}^2$	$(C_3{}^2)^{-1} = C_3$
e	e	σ_1	σ_2	σ_3	$C_3{}^2$	C_3
$\boldsymbol{\sigma}_1$	σ_1	e	C_3	$C_3{}^2$	σ_3	σ_2
$\boldsymbol{\sigma}_2$	σ_2	$C_3{}^2$	e	C_3	σ_1	σ_3
$\boldsymbol{\sigma}_3$	σ_3	C_3	$C_3{}^2$	e	σ_2	σ_1
C_3	C_3	σ_3	σ_1	σ_2	e	$C_3{}^2$
$C_3{}^2$	$C_3{}^2$	σ_2	σ_3	σ_1	C_3	e

$D^R(g)^i{}_j$ is obtained by setting 1 to all occurrences of g in the above table:

$$D^R(e) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad D^R(\sigma_1) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

$$D^R(\sigma_2) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad D^R(\sigma_3) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

$$D^R(C_3) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \qquad D^R\left(C_3{}^2\right) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Note that each row & column has only one 1.

The character table is

C_{3v}	e	$3\,\sigma$	$2\,C_3$
χ^1	1	1	1
χ^2	1	−1	1
χ^3	2	0	−1
χ^R	6	0	0

Thus,

$$\chi_1{}^\dagger \cdot \chi^R = 1\cdot 6 + 3\,(1\cdot 0) + 2\,(1\cdot 0) = 6 \qquad \Rightarrow \qquad a_1 = 1$$
$$\chi_2{}^\dagger \cdot \chi^R = 1\cdot 6 + 3\,(-1\cdot 0) + 2\,(1\cdot 0) = 6 \qquad \Rightarrow \qquad a_2 = 1$$
$$\chi_3{}^\dagger \cdot \chi^R = 2\cdot 6 + 3\,(0\cdot 0) + 2\,(-1\cdot 0) = 12 \qquad \Rightarrow \qquad a_3 = 2$$

which confirms the theorem

$$D^R = n_\mu\, D^\mu$$

ie., each IR appears n_μ times in D^R.

■ $P^j{}_{\mu i}$

Consider the projection operators

$$P^j{}_{\mu i} = \frac{n_\mu}{n_G} \sum_g D^{-1}{}_\mu(g)^j{}_i\, U(g)$$

For $\mu = 1$,

$$P_1 = \frac{1}{6}\left[\, e + \sigma_1 + \sigma_2 + \sigma_3 + C_3 + C_3{}^2 \,\right] \qquad (\text{ label } i = j = 1 \text{ suppressed })$$

For $\mu = 2$,

$$P_2 = \frac{1}{6}\left[\ e - \sigma_1 - \sigma_2 - \sigma_3 + C_3 + C_3{}^2\ \right]$$

For $\mu = 3$,

$$D^3(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$D^3(\sigma_1) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \qquad D^3(\sigma_2) = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \qquad D^3(\sigma_3) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$D^3(C_3) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \qquad D^3\left(C_3{}^2\right) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

$$P^1{}_{31} = \frac{1}{3}\left[\ e + \frac{1}{2}\,\sigma_1 + \frac{1}{2}\,\sigma_2 - \sigma_3 - \frac{1}{2}\,C_3 - \frac{1}{2}\,C_3{}^2\ \right]$$

$$= \frac{1}{3}\begin{pmatrix} 1 + \frac{1}{4} + \frac{1}{4} + 1 + \frac{1}{4} + \frac{1}{4} & 0 + \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} - 0 + \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} \\ 0 + \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} - 0 - \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} & 1 - \frac{1}{4} - \frac{1}{4} - 1 + \frac{1}{4} + \frac{1}{4} \end{pmatrix}$$

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

$$P^1{}_{32} = \frac{1}{3}\left[\ \frac{\sqrt{3}}{2}\,\sigma_1 - \frac{\sqrt{3}}{2}\,\sigma_2 + \frac{\sqrt{3}}{2}\,C_3 - \frac{\sqrt{3}}{2}\,C_3{}^2\ \right]$$

$$= \frac{1}{3}\begin{pmatrix} \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} & \frac{3}{4} + \frac{3}{4} - \frac{3}{4} - \frac{3}{4} \\ \frac{3}{4} + \frac{3}{4} + \frac{3}{4} + \frac{3}{4} & -\frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} \end{pmatrix}$$

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

$$P^2{}_{31} = \frac{1}{3}\left[\ \frac{\sqrt{3}}{2}\,\sigma_1 - \frac{\sqrt{3}}{2}\,\sigma_2 - \frac{\sqrt{3}}{2}\,C_3 + \frac{\sqrt{3}}{2}\,C_3{}^2\ \right]$$

$$= \frac{1}{3}\begin{pmatrix} \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} & \frac{3}{4} + \frac{3}{4} + \frac{3}{4} + \frac{3}{4} \\ \frac{3}{4} + \frac{3}{4} - \frac{3}{4} - \frac{3}{4} & -\frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} \end{pmatrix}$$

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

$$P^2{}_{32} = \frac{1}{3}\left[\ e - \frac{1}{2}\,\sigma_1 - \frac{1}{2}\,\sigma_2 + \sigma_3 - \frac{1}{2}\,C_3 - \frac{1}{2}\,C_3{}^2\ \right]$$

$$= \frac{1}{3}\begin{pmatrix} 1 - \frac{1}{4} - \frac{1}{4} - 1 + \frac{1}{4} + \frac{1}{4} & 0 - \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} + 0 + \frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4} \\ 0 - \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} + 0 - \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4} & 1 + \frac{1}{4} + \frac{1}{4} + 1 + \frac{1}{4} + \frac{1}{4} \end{pmatrix}$$

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

It's clear that $P^i{}_{\mu\, j}$ is a projector.

Actually, for an orthonormal basis { $\hat{e}^{\mu}{}_i$ }, we can write

$$P^i{}_{\mu\, j} = \left| \bar{e}^{\mu}{}_j \right\rangle \left\langle\, e_{\mu}{}^i \right|$$

The matrix elements of $P^i{}_{\mu\, j}$ then become

$$\left[P^i{}_{\mu\, j}\right]^l{}_m = \left\langle\, e_{\mu}{}^l \right| P^i{}_{\mu\, j} \left| \bar{e}^{\mu}{}_m \right\rangle$$

$$= \left\langle\, e_{\mu}{}^l \right| \left. \bar{e}^{\mu}{}_j \right\rangle \left\langle\, e_{\mu}{}^i \right| \left. \bar{e}^{\mu}{}_m \right\rangle$$

$$= \delta^l{}_j\, \delta^i{}_m$$

$$P_{\mu} = P_{\mu}{}^i{}_i = \frac{n_{\mu}}{n_G} \sum_g D^{-1}{}_{\mu}(g)^i{}_i\, U(g)$$

$$= \frac{n_{\mu}}{n_G} \sum_g \chi_{\mu}\left(g^{-1}\right) U(g)$$

$$P_3 = \frac{1}{3}\left[\, 2\, e - C_3 - C_3{}^2 \,\right]$$

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

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

For $\mu = 4$,

$$\mathrm{D}^4\,(\mathrm{e}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$D^4(\sigma_1) = \begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix} \qquad D^4(\sigma_2) = \begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix} \qquad D^4(\sigma_3) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$D^4(C_3) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} \qquad D^4\left(C_3{}^2\right) = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$$

$$P^1{}_{41} = \frac{1}{3}\left[\, e + \sigma_1 - \sigma_2 - C_3 \,\right]$$

$$= \frac{1}{3} \begin{pmatrix} 1 + 1 + 1 - 0 & 0 - 1 - 0 + 1 \\ 0 + 0 + 1 - 1 & 1 - 1 - 1 + 1 \end{pmatrix}$$

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

$$P^1{}_{42} = \frac{1}{3}\left[\, -\sigma_1 + \sigma_3 + C_3 - C_3{}^2 \,\right]$$

$$= \frac{1}{3}\begin{pmatrix} -1+0+0+1 & 1+1-1-1 \\ 0+1+1+1 & 1+0-1-0 \end{pmatrix}$$

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

$$P^2{}_{41} = \frac{1}{3}\left[-\sigma_2 + \sigma_3 - C_3 + C_3{}^2 \right]$$

$$= \frac{1}{3}\begin{pmatrix} 1+0-0-1 & 0+1+1+1 \\ 1+1-1-1 & -1+0+1+0 \end{pmatrix}$$

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

$$P^2{}_{42} = \frac{1}{3}\left[e - \sigma_1 + \sigma_2 - C_3{}^2 \right]$$

$$= \frac{1}{3}\begin{pmatrix} 1-1-1+1 & 0+1+0-1 \\ 0+0-1+1 & 1+1+1+0 \end{pmatrix}$$

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

■ IBs

By construction,

$\{\hat{e}_1, \hat{e}_2\}$ is IB for D^3

$\{u_1, u_2\}$ is IB for D^4.

Given $\hat{e}_1$, the effects of $P^i{}_{4j}$ are:

$$P^1{}_{41}\, \hat{e}_1 = \frac{1}{3}[\, e + \sigma_1 - \sigma_2 - C_3 \,]\, \hat{e}_1$$

$$= \frac{1}{3}\left[\hat{e}_1 + \left(\frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \right) - \left(\frac{1}{2}\hat{e}_1 - \frac{\sqrt{3}}{2}\hat{e}_2 \right) - \left(-\frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \right) \right]$$

$$= \frac{1}{3}\left[\frac{3}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \right]$$

$$= \frac{1}{\sqrt{3}}\left[\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2 \right]$$

$$= -\frac{1}{\sqrt{3}}\hat{u}_1$$

$$P^1{}_{42}\, \hat{e}_1 = \frac{1}{3}\left[-\sigma_1 + \sigma_3 + C_3 - C_3{}^2 \right] \hat{e}_1$$

$$= \frac{1}{3}\left[-\left(\frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \right) - \hat{e}_1 + \left(-\frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \right) - \left(-\frac{1}{2}\hat{e}_1 - \frac{\sqrt{3}}{2}\hat{e}_2 \right) \right]$$

$$= \frac{1}{3}\left[-\frac{3}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2 \right]$$

$$= \frac{1}{\sqrt{3}}\left[-\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2 \right]$$

$$= -\frac{1}{\sqrt{3}}\hat{u}_2$$

And similarly for the other terms of the form $P^{i}{}_{4\,j}\ \hat{e}_k$.

Note that in the $\hat{e}_i$ basis,

$$\begin{aligned} P^1{}_{41} &= \frac{1}{3}[\ e + \sigma_1 - \sigma_2 - C_3\ ] \\ &= \frac{1}{3}\begin{pmatrix} 1+\frac{1}{2}-\frac{1}{2}+\frac{1}{2} & 0+\frac{\sqrt{3}}{2}+\frac{\sqrt{3}}{2}+\frac{\sqrt{3}}{2} \\ 0+\frac{\sqrt{3}}{2}+\frac{\sqrt{3}}{2}-\frac{\sqrt{3}}{2} & 1-\frac{1}{2}+\frac{1}{2}+\frac{1}{2} \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{1}{2\sqrt{3}} & \frac{1}{2} \end{pmatrix} \end{aligned}$$

which is not of the simple form as in the $\hat{u}_i$ basis.

Nevertheless,

$$\begin{aligned} P^1{}_{41}\ \hat{e}_1 &= \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{1}{2\sqrt{3}} & \frac{1}{2} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2\sqrt{3}} \end{pmatrix} \\ &= \frac{1}{2}\hat{e}_1 + \frac{1}{2\sqrt{3}}\hat{e}_2 \\ &= -\frac{1}{\sqrt{3}}\hat{u}_1 \end{aligned}$$

as expected.

Recalling,

$$S\, D^3(g)\, S^{-1} = D^4(g)$$

$$\hat{u}_i = \hat{e}_j \left(S^{-1}\right)^j{}_i \qquad \hat{e}_i = \hat{u}_j\, S^j{}_i$$

$$S^{-1} = \begin{pmatrix} -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\ -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \qquad S = \begin{pmatrix} -\frac{1}{\sqrt{3}} & -1 \\ \frac{1}{\sqrt{3}} & -1 \end{pmatrix}$$

implies

$$S\, D^3(g)\, S^{-1} = D^4(g)$$

Alternatively, we can also write:

$$\begin{aligned} P^1{}_{41}\ \hat{e}_1 &= \frac{1}{3}[\ e + \sigma_1 - \sigma_2 - C_3\ ]\left(-\frac{1}{\sqrt{3}}\hat{u}_1 + \frac{1}{\sqrt{3}}\hat{u}_2\right) \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} \\ &= -\frac{1}{\sqrt{3}}\hat{u}_1 \end{aligned}$$

$$P^1{}_{42}\,\hat{e}_1 = \frac{1}{3}\left[\,-\sigma_1 + \sigma_3 + C_3 - C_3{}^2\,\right]\left(-\frac{1}{\sqrt{3}}\,\hat{u}_1 + \frac{1}{\sqrt{3}}\,\hat{u}_2\right)$$

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

$$= -\frac{1}{\sqrt{3}}\,\hat{u}_2$$

■ NH_3

Atoms of the NH_3 molecule occupy the vertices of a tetrahedron.
The 3 H atoms, labelled 1, 2, & 3, form at the base an equilateral triangle.
The N atom, labelled 0, occupies the apex.

The main cohesion is due to the 3 valence bonds between N and each of the H atoms.
Thus, we can neglect the H-H interactions.

Consider the bonding due only to the *s* electrons.
Let $|\,l\,\rangle$ be the *s* state at the *l*th atom.
The basis functions are $\{\,|\,l\,\rangle,\ l = 0, 1, 2, 3\,\}$.
The matrix elements $H_{l\,m} = \langle\, l\,|\,H\,|\,m\,\rangle$ are

$$H_{00} = \epsilon_N \qquad H_{i\,i} = \epsilon_H \qquad i,\ j = 1, 2, 3$$
$$H_{0\,i} = H_{i\,0} = V \qquad H_{i\,j} = W$$

ie

$$H = \begin{pmatrix} \epsilon_N & V & V & V \\ V & \epsilon_H & W & W \\ V & W & \epsilon_H & W \\ V & W & W & \epsilon_H \end{pmatrix}$$

The basis form a 4-D rep for $C_{3\,v}$.
Actually, since none of the symmetry operations mixes N with H, $|\,0\,\rangle$ by itself is an 1-D IB.

The character table is

$C_{3\,v}$	e	$3\,\sigma$	$2\,C_3$
χ^1	1	1	1
χ^2	1	−1	1
χ^3	2	0	−1
χ^N	1	1	1
χ^{H_3}	3	1	0
χ^{NH_3}	4	2	1

Obviously,

$$\chi^N = \chi^1$$
$$\chi^{H_3} = \chi^1 + \chi^3$$
$$\chi^{NH_3} = 2\,\chi^1 + \chi^3$$

The IBs for H_3 are

D^1 : $P^1 | 1 \rangle = \frac{1}{6}\left[e + \sigma_1 + \sigma_2 + \sigma_3 + C_3 + C_3{}^2 \right] | 1 \rangle$

$= \frac{1}{6}[| 1 \rangle + | 1 \rangle + | 3 \rangle + | 2 \rangle + | 2 \rangle + | 3 \rangle]$

$= \frac{1}{3} [| 1 \rangle + | 2 \rangle + | 3 \rangle]$

Normalized version:

$$\left| e^1 \right\rangle = \frac{1}{\sqrt{3}} [| 1 \rangle + | 2 \rangle + | 3 \rangle]$$

D^3 :

$P^1{}_{31} | 1 \rangle = \frac{1}{3}\left[e + \frac{1}{2} \sigma_1 + \frac{1}{2} \sigma_2 - \sigma_3 - \frac{1}{2} C_3 - \frac{1}{2} C_3{}^2 \right] \left| 1 \right\rangle$

$= \frac{1}{3}\left[| 1 \rangle + \frac{1}{2} | 1 \rangle + \frac{1}{2} | 3 \rangle - | 2 \rangle - \frac{1}{2} | 2 \rangle - \frac{1}{2} | 3 \rangle \right]$

$= \frac{1}{2} [| 1 \rangle - | 2 \rangle]$

Normalized version:

$$\left| e^3{}_1 \right\rangle = \frac{1}{\sqrt{2}} [| 1 \rangle - | 2 \rangle]$$

$P^1{}_{32} | 1 \rangle = \frac{1}{3}\left[\frac{\sqrt{3}}{2} \sigma_1 - \frac{\sqrt{3}}{2} \sigma_2 + \frac{\sqrt{3}}{2} C_3 - \frac{\sqrt{3}}{2} C_3{}^2 \right]$

$= \frac{1}{3}\left[\frac{\sqrt{3}}{2} | 1 \rangle - \frac{\sqrt{3}}{2} | 3 \rangle + \frac{\sqrt{3}}{2} | 2 \rangle - \frac{\sqrt{3}}{2} | 3 \rangle \right]$

$= \frac{1}{2\sqrt{3}} [| 1 \rangle + | 2 \rangle - 2 | 3 \rangle]$

Normalized version:

$$\left| e^3{}_2 \right\rangle = \frac{1}{\sqrt{6}} [| 1 \rangle + | 2 \rangle - 2 | 3 \rangle]$$

$P^2{}_{31} | 1 \rangle = \frac{1}{3}\left[\frac{\sqrt{3}}{2} \sigma_1 - \frac{\sqrt{3}}{2} \sigma_2 - \frac{\sqrt{3}}{2} C_3 + \frac{\sqrt{3}}{2} C_3{}^2 \right] | 1 \rangle$

$= \frac{1}{3}\left[\frac{\sqrt{3}}{2} | 1 \rangle - \frac{\sqrt{3}}{2} | 3 \rangle - \frac{\sqrt{3}}{2} | 2 \rangle + \frac{\sqrt{3}}{2} | 3 \rangle \right]$

$= \frac{1}{2\sqrt{3}} [| 1 \rangle - | 2 \rangle]$

$P^2{}_{32} | 1 \rangle = \frac{1}{3}\left[e - \frac{1}{2} \sigma_1 - \frac{1}{2} \sigma_2 + \sigma_3 - \frac{1}{2} C_3 - \frac{1}{2} C_3{}^2 \right] | 1 \rangle$

$= \frac{1}{3}\left[| 1 \rangle - \frac{1}{2} | 1 \rangle - \frac{1}{2} | 3 \rangle + | 2 \rangle - \frac{1}{2} | 2 \rangle - \frac{1}{2} | 3 \rangle \right]$

$= \frac{1}{6} [| 1 \rangle + | 2 \rangle - 2 | 3 \rangle]$

$$P_3 |1\rangle = \frac{1}{3}\left[2e - C_3 - C_3{}^2\right]|1\rangle$$
$$= \frac{1}{3}[2|1\rangle - |2\rangle - |3\rangle]$$

$$P_3 |2\rangle = \frac{1}{3}\left[2e - C_3 - C_3{}^2\right]|2\rangle$$
$$= \frac{1}{3}[2|2\rangle - |3\rangle - |1\rangle]$$

To summarizem, the IBs are

$$\left|u^1\right\rangle = |0\rangle$$
$$\left|e^1\right\rangle = \frac{1}{\sqrt{3}}[|1\rangle + |2\rangle + |3\rangle]$$
$$\left|e^3{}_1\right\rangle = \frac{1}{\sqrt{2}}[|1\rangle - |2\rangle]$$
$$\left|e^3{}_2\right\rangle = \frac{1}{\sqrt{6}}[|1\rangle + |2\rangle - 2|3\rangle]$$

The transformation between bases is

$$\left(\left|u^1\right\rangle, \left|e^1\right\rangle, \left|e^3{}_1\right\rangle, \left|e^3{}_2\right\rangle\right)$$
$$= (|0\rangle, |1\rangle, |2\rangle, |3\rangle)\, S$$
$$= (|0\rangle, |1\rangle, |2\rangle, |3\rangle)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{3}} & 0 & -\frac{2}{\sqrt{6}} \end{pmatrix}$$

$$S^{-1} = S^{\dagger} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} \end{pmatrix}$$

In the IBs, H becomes

$$S^{-1}\,H\,S=\begin{pmatrix}1&0&0&0\\0&\frac{1}{\sqrt{3}}&\frac{1}{\sqrt{3}}&\frac{1}{\sqrt{3}}\\0&\frac{1}{\sqrt{2}}&-\frac{1}{\sqrt{2}}&0\\0&\frac{1}{\sqrt{6}}&\frac{1}{\sqrt{6}}&-\frac{2}{\sqrt{6}}\end{pmatrix}\begin{pmatrix}\epsilon_N&V&V&V\\V&\epsilon_H&W&W\\V&W&\epsilon_H&W\\V&W&W&\epsilon_H\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&\frac{1}{\sqrt{3}}&\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{6}}\\0&\frac{1}{\sqrt{3}}&-\frac{1}{\sqrt{2}}&\frac{1}{\sqrt{6}}\\0&\frac{1}{\sqrt{3}}&0&-\frac{2}{\sqrt{6}}\end{pmatrix}$$

$$=\begin{pmatrix}1&0&0&0\\0&\frac{1}{\sqrt{3}}&\frac{1}{\sqrt{3}}&\frac{1}{\sqrt{3}}\\0&\frac{1}{\sqrt{2}}&-\frac{1}{\sqrt{2}}&0\\0&\frac{1}{\sqrt{6}}&\frac{1}{\sqrt{6}}&-\frac{2}{\sqrt{6}}\end{pmatrix}\begin{pmatrix}\epsilon_N&\sqrt{3}\,V&0&0\\V&\frac{1}{\sqrt{3}}\epsilon_H+\frac{2}{\sqrt{3}}W&\frac{1}{\sqrt{2}}\epsilon_H-\frac{1}{\sqrt{2}}W&\frac{1}{\sqrt{6}}\epsilon_H-\frac{1}{\sqrt{6}}W\\V&\frac{1}{\sqrt{3}}\epsilon_H+\frac{2}{\sqrt{3}}W&-\frac{1}{\sqrt{2}}\epsilon_H+\frac{1}{\sqrt{2}}W&\frac{1}{\sqrt{6}}\epsilon_H-\frac{1}{\sqrt{6}}W\\V&\frac{1}{\sqrt{3}}\epsilon_H+\frac{2}{\sqrt{3}}W&0&-\frac{2}{\sqrt{6}}\epsilon_H+\frac{2}{\sqrt{6}}W\end{pmatrix}$$

$$=\begin{pmatrix}\epsilon_N&\sqrt{3}\,V&0&0\\\sqrt{3}\,V&\epsilon_H+2\,W&0&0\\0&0&\epsilon_H-W&0\\0&0&0&\epsilon_H-W\end{pmatrix}$$