# Determination of The Trace of a Matrix

* Working with The $C_{2h}$ point group:

$$E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \sigma_h = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$C_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad i = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Block-diagonalization gives out

$$E = \left[\begin{array}{c|c|c} 1 & 0 & 0 \\ \hline 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right]$$

$\sigma_h$, $C_2$ and $i$ are dealt with in a similar way.

Thus:

| $C_{2h}$ | $E$ | $C_2$ | $i$ | $\sigma_h$ |
|---|---|---|---|---|
| $\Gamma^{red}$ | 3 | -1 | -3 | 1 |
| $\Gamma^1$ | 1 | -1 | -1 | 1 |
| $\Gamma^2$ | 1 | -1 | -1 | 1 |
| $\Gamma^3$ | 1 | 1 | -1 | -1 |

It should be noticed that

$$\Gamma^{red} = \Gamma^1 \oplus \Gamma^2 \oplus \Gamma^3$$

Also, each $\Gamma^n$ where $n = 1, 2,$ or $3$ has unique characters with respect to symmetry elements.

* Working with the $C_{3v}$ point group. (a little more complicated system).

This group has six symmetry elements with six distinct matrices ($E$, $C_3$, $C_3^2$, $\sigma_v'$, $\sigma_v''$, $\sigma_v'''$)

| $C_{3v}$ | $E$ | $C_3$ | $C_3^2$ | $\sigma_v'$ | $\sigma_v''$ | $\sigma_v'''$ |
|---|---|---|---|---|---|---|
| $\Gamma^{red}$ | 3 | 0 | 0 | 1 | 1 | 1 |
| $\Gamma^1$ | 1 | 1 | 1 | 1 | 1 | 1 |
| $\Gamma^2$ | 2 | -1 | -1 | 0 | 0 | 0 |

$$\Gamma^{red} = \Gamma^1 \oplus \Gamma^2$$

Further treatment using the great orthogonality theorem must yield that

① $\sum_{\hat{R}} \Gamma^1 \Gamma^2 = 0$ , and

② $\sum_{\hat{R}} \Gamma^1 \Gamma^1 = \sum_{\hat{R}} \Gamma^2 \Gamma^2 = g$ (where $g$ is the number of members)

Checking for ① & ② :

$$\sum_{\hat{R}} \Gamma^1 \Gamma^2 = 1 \cdot 2 + 1(-1) + 1(-1) + 1(0) + 1(0) + 1(0)$$
$$= 2 + (-2) + 0 = 0$$

$$\sum_{\hat{R}} \Gamma^1 \Gamma^1 = 1 + 1 + 1 + 1 + 1 + 1 = 6$$

$$\sum_{\hat{R}} \Gamma^2 \Gamma^2 = 2(2) + (-1)(-1) + (-1)(-1) + 0 + 0 + 0 = 6$$

In order to determine the 3rd irreducible representation (Notice: the required number of irreducible representations is determined from the orthogonality theorem), we use determinants to evaluate the traces for the reducible matrices:

For example for the 2x2 matrices:

$$E = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \Rightarrow |E| = 1 - 0 = 1$$

$$C_3 = \begin{bmatrix} -1/2 & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -1/2 \end{bmatrix} \Rightarrow |C_3| = \frac{1}{4} + \frac{3}{4} = 1$$

$$\sigma_v''' = \begin{bmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix} \Rightarrow \sigma_v''' = -\frac{1}{4} - \frac{3}{4} = -1$$

Adding the third irreducible representation to the previous two gives:

| $C_{3v}$ | $E$ | $C_3$ | $C_3^2$ | $\sigma_v'$ | $\sigma_v''$ | $\sigma_v'''$ |
|---|---|---|---|---|---|---|
| $\Gamma^3$ | 1 | 1 | 1 | −1 | −1 | −1 |