APPLICATION OF THE GREAT ORTHOGONALITY THEOREM: EXAMPLES

The set of matrices in the cartesian representations for C_{3v} form a *reducible representation* comprised of the following 2×2 and 1×1 irreducible representations:

$$\underset{v_1 \quad v_2}{} \quad \underline{\Gamma}_1(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \underline{\Gamma}_1(C_3) = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} \quad \underline{\Gamma}_1(C_3^2) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$$

$$\underline{\Gamma}_1(\sigma_v') = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \underline{\Gamma}_1(\sigma_v'') = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix} \quad \underline{\Gamma}_1(\sigma_v''') = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix}$$

and

v_3

$$\underline{\Gamma}_2(E) = 1 \quad \underline{\Gamma}_2(C_3) = 1 \quad \underline{\Gamma}_2(C_3^2) = 1 \quad \underline{\Gamma}_2(\sigma_v') = 1 \quad \underline{\Gamma}_2(\sigma_v'') = 1 \quad \underline{\Gamma}_2(\sigma_v''') = 1$$

G.O.T.: $$\sum_{\Re=1}^{h} (\Gamma_1^*(\hat{\Re}))_{mn} (\Gamma_j(\hat{\Re}))_{m'n'} = \frac{h}{\sqrt{\ell_i \ell_j}} \delta_{ij} \delta_{mm'} \delta_{nn'}$$

Case $\vec{v}_2 \cdot \vec{v}_2$: i = 1, m = 1, n = 2; j = 1, m' = 1, n' = 2

$$0 \cdot 0 + \frac{\sqrt{3}}{2} \cdot \frac{\sqrt{3}}{2} + \left(-\frac{\sqrt{3}}{2}\right)\left(-\frac{\sqrt{3}}{2}\right) + 0 \cdot 0 + \frac{\sqrt{3}}{2} \cdot \frac{\sqrt{3}}{2} + \left(-\frac{\sqrt{3}}{2}\right)\left(-\frac{\sqrt{3}}{2}\right) = \frac{12}{4} = \frac{6}{2}$$

E $\quad C_3 \quad C_3^2 \quad \sigma_v' \quad \sigma_v'' \quad \sigma_v'''$

Q.E.D.

$$1 \cdot 1 + -1/2 \cdot 1 + -1/2 \cdot 1 + 1 \cdot 1 + -1/2 \cdot 1 + -1/2 \cdot 1 = 0$$

Case $\vec{v}_1 \cdot \vec{v}_3$: i = 1, m = 1, n = 1; j = 2, m' = 1, n' = 1

Case $\vec{v}_1 \cdot \vec{v}_2$: i = 1, m = 1, n = 1; j = 1, m' = 1, n' = 2

$$1 \cdot 0 + \left(-\frac{1}{2}\right)\left(\frac{\sqrt{3}}{2}\right) + \left(-\frac{1}{2}\right)\left(-\frac{\sqrt{3}}{2}\right) + (1)(0) + \left(-\frac{1}{2}\right)\left(\frac{\sqrt{3}}{2}\right) + \left(-\frac{1}{2}\right)\left(-\frac{\sqrt{3}}{2}\right) = 0 \leftarrow \text{Q.E.D.}$$

E $\quad C_3 \quad C_3^2 \quad \sigma' \quad \sigma_v'' \quad \sigma_v'''$