Character Tables: Procedure for Derivation

- delineate symmetry elements, classes
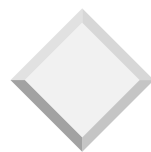- # of I.R.'s = # of Classes
- dimensions of I.R.'s:

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

- orthogonality and normalization of I.R.'s

$$\sum_R [\chi_i(R)]^2 = h \quad ; \quad \sum_R \chi_i(R)\chi_j(R) = 0 \text{ when } i \neq j$$

- Mulliken Symbols
- bases for I.R.'s, linear and bilinear forms

Derivation of Character Tables; Examples

★ C_{2v} - easy!

★ C_{4v} - an example with a 2-dim. I.R.

★ D_{3h} vs. D_{3d}
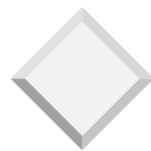
★ O_h - Divide and Conquer

★ $O_h = O \times C_i$

A Crucial Practical Relationship

★ Any reducible rep. can be put in block-diagonal form by some similarity transformation (i.e., appropriate choice of basis)

★ Let a_j be the # of times the jth irred. rep. occurs. The character of the red. rep. is then:

$$\chi(R) = \sum_j a_j \chi_j(R)$$

★ A formula for a_i is: $\quad a_i = \frac{1}{h}\sum_R \chi(R)\chi_i(R)$

Examples

★ Find the characters of the reducible representation obtained using the four hydrogen 1s orbitals of methane as a basis — then find the irred. reps. spanned by this rep.

★ Follow the same procedure using the twelve CO π^* orbitals of $Cr(CO)_6$ as a basis.

★ Follow the same procedure using the six CO stretching vibrations of $Cr(CO)_6$ as a basis.