

### The Direct Product

- form the product  $A_2 \otimes B_1$  for the  $C_{2v}$  point group explicitly by multiplying the characters, and check your answer by using the "rules" in your hand-out.

| $C_{2v}$          | $E$ | $C_2$ | $\sigma_v$ | $\sigma'_v$          |
|-------------------|-----|-------|------------|----------------------|
| $A_2$             | 1   | 1     | -1         | -1                   |
| $B_2$             | 1   | -1    | -1         | 1                    |
| $A_2 \otimes B_2$ | 1   | -1    | 1          | -1 $\Rightarrow B_1$ |

- $A_2 \otimes B_1 = B_2$  since  $A \otimes B = B$  and  $1 \otimes 2 = 2$

### Using Symmetry to Determine Infrared Activity

- determine if excitation of the  $B_2$  vibration of  $H_2O$  is allowed for IR spectra:
  - For  $\Gamma^f = A_1$  we require the cross product below to contain the  $A_1$  IR:

$$\left\{ \Gamma^{\langle \chi_f |} \otimes \Gamma^{|\chi_i \rangle} \right\} \otimes \Gamma^\lambda = \{B_2 \otimes A_1\} \otimes \begin{bmatrix} B_1 \\ B_2 \\ A_1 \end{bmatrix} = B_2 \otimes \begin{bmatrix} B_1 \\ B_2 \\ A_1 \end{bmatrix} = \{A_2, A_1, B_1\}$$

- $A_1$  is present and so the  $B_2$  vibration is allowed  $\Rightarrow$  we will see a  $B_2$  peak in the infrared spectrum of water

### Using Symmetry to Determine Raman Activity

- determine if excitation of the  $B_2$  vibration is allowed for RAMAN spectra:

$$\left\{ \Gamma^{\langle \chi_f |} \otimes \Gamma^{|\chi_i \rangle} \right\} \otimes \Gamma^\alpha = \{B_2 \otimes A_1\} \otimes \begin{bmatrix} A_1 \\ B_1 \\ A_2 \\ B_2 \end{bmatrix} = B_2 \otimes \begin{bmatrix} A_1 \\ B_1 \\ A_2 \\ B_2 \end{bmatrix} = \{B_2, A_2, B_1, A_1\}$$

- $A_1$  is present and so the  $B_2$  vibration is allowed  $\Rightarrow$  we will see a  $B_2$  peak in the infrared spectrum of water