Reducing Reducible Representations

We need to use the reduction formula: $$a_p = \left(\frac{1}{g}\right)\sum_R n_R \cdot \chi(R) \cdot \chi_p(R)$$

Where a_p is the number of times the irreducible representation, p, occurs in any reducible representation.

g is the number of symmetry operations in the group

$\chi(R)$ is character of the **reducible** representation

$\chi_p(R)$ is character of the **irreducible** representation

n_R is the number of operations in the class

C_{2v}	1E	$1C_2$	$1\sigma_{(xz)}$	$1\sigma_{(yz)}$		
A_1	+1	+1	+1	+1	T_z	x^2, y^2, z^2
A_2	+1	+1	-1	-1	R_z	xy
B_1	+1	-1	+1	-1	T_x, R_x	xz
B_2	+1	-1	-1	+1	T_y, R_y	yz

For C_{2v} ; g = 4 and n_R = 1 for all operations

C_{2v}	E	C_2	$\sigma_{(xz)}$	$\sigma_{(yz)}$
Γ_{3n}	+9	-1	+1	3

$$a_p = \left(\frac{1}{g}\right)\sum_R n_R.\chi(R).\chi_p(R)$$

$$a_{A_1} = (1/4)[\ (1x9x1) + (1x\text{-}1x1) + (1x1x1) + (1x3x1)] = (12/4) = 3$$

$$a_p = \left(\frac{1}{g}\right)\sum_R n_R.\chi(R).\chi_p(R)$$

C_{2v}	E	C_2	$\sigma_{(xz)}$	$\sigma_{(yz)}$
Γ_{3n}	+9	-1	+1	3

a_{A_1} = (1/4)[(1x9x1) + (1x-1x1) + (1x1x1) + (1x3x1)] = (12/4) =3

a_{A_2} = (1/4)[(1x9x1) + (1x-1x1) + (1x1x-1) + (1x3x-1)] = (4/4) =1

a_{B_1} = (1/4)[(1x9x1) + (1x-1x-1) + (1x1x1) + (1x3x-1)] = (8/4) =2

a_{B_2} = (1/4)[(1x9x1) + (1x-1x-1) + (1x1x-1) + (1x3x1)] = (12/4) =3

$$\boxed{\Gamma_{3n} = 3A_1 + A_2 + 2B_1 + 3B_2}$$

Reducing Reducible Representations

$$a_{A_1} = (1/4)[\ (1\text{x}\mathbf{9}\text{x}1) + (1\text{x-}\mathbf{1}\text{x}1) + (1\text{x}\mathbf{1}\text{x}1) + (1\text{x}\mathbf{3}\text{x}1)] = (12/4) = 3$$

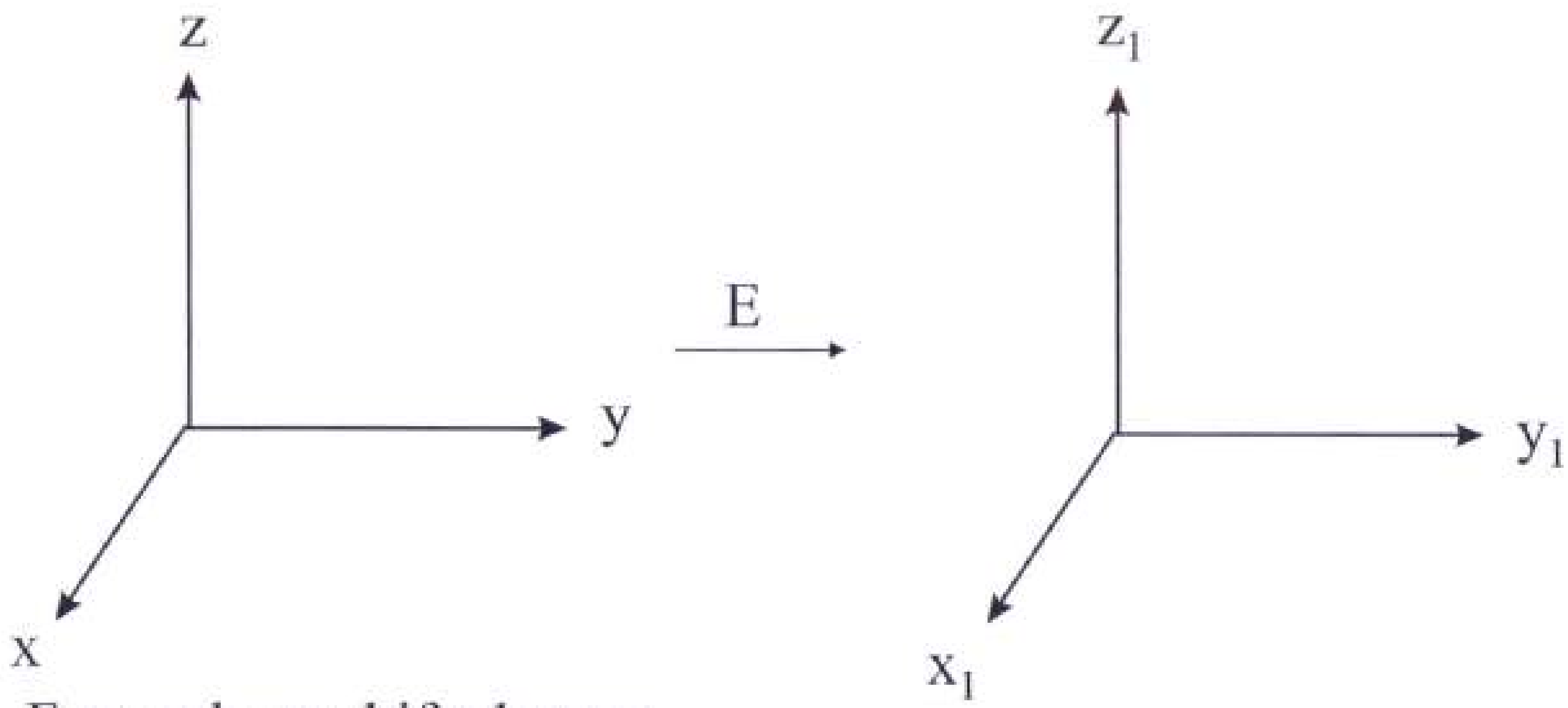
The terms in blue represent contributions from the **un-shifted** atoms **Only** these actually contribute to the trace.

If we concentrate only on these un-shifted atoms we can simplify the problem greatly.

For SO_2 (**9** = 3 x *3*) (**-1** = 1 x *–1*) (**1** = 1 x *1*) and (**3** = 3 x *1*)

Number of un-shifted atoms ***Contribution from these atoms***

Identity E

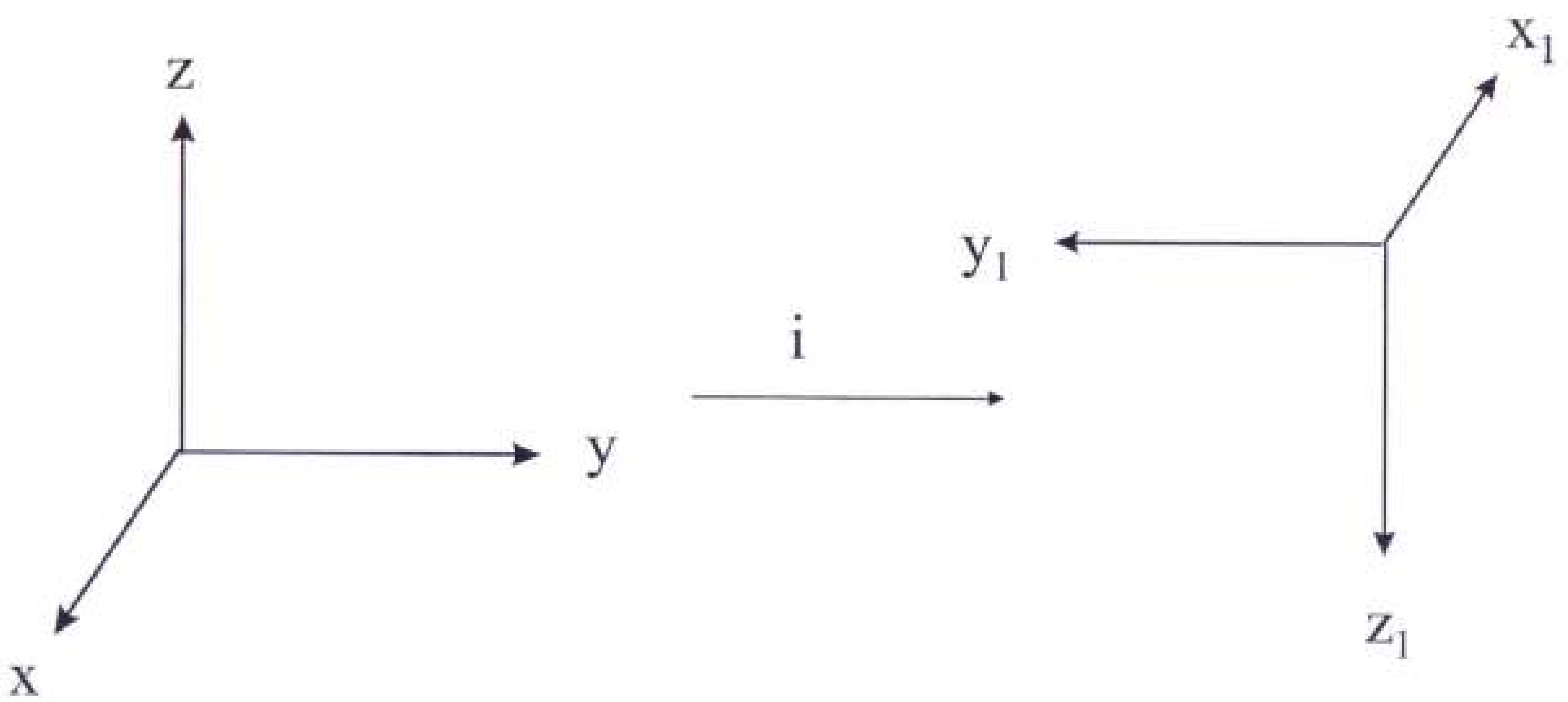


For each un-shifted atom

$$\begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} . \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$\chi(E) = +3$

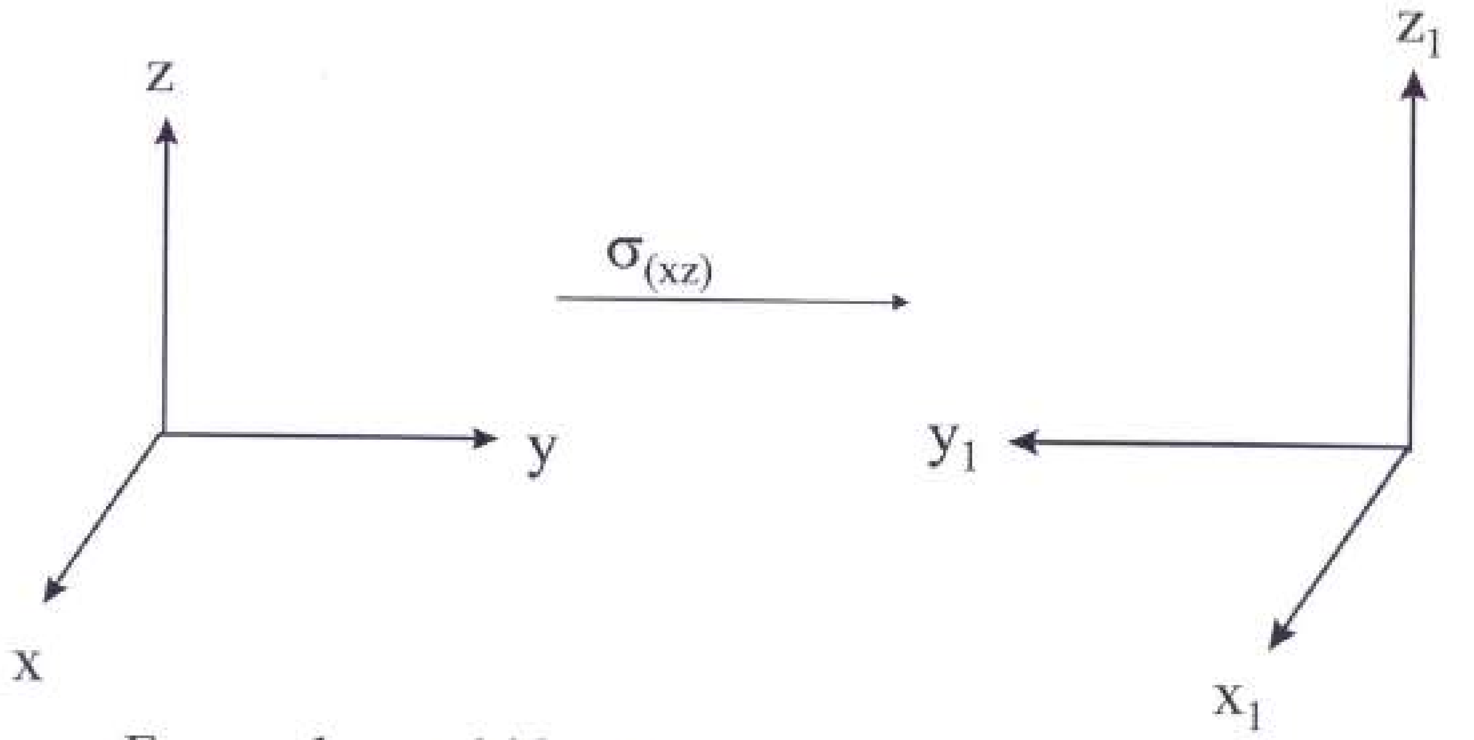
Inversion i



For each un-shifted atom

$$\begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} . \begin{bmatrix} x \\ y \\ z \end{bmatrix} \qquad \chi(i) = -3$$

Reflection $\sigma_{(xz)}$ (Others are same except location of –1 changes)



For each un-shifted atom

$$\begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} . \begin{bmatrix} x \\ y \\ z \end{bmatrix} \qquad \chi(\sigma_{(xz)}) = +1$$