(disregard handout from 4/11)

Chemistry 5b
4/14/03

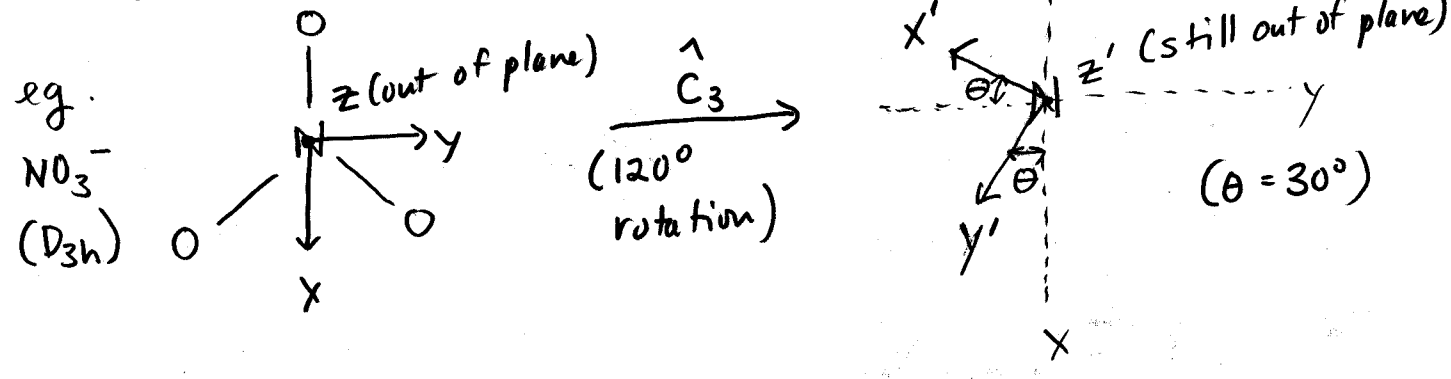
Predicting Characters for Symmetry Operations with a Given Basis Set

The rules so far:

- Unchanged ⇒ +1 to character
- Changes sign ⇒ −1 to character (i.e. rotated 180°)
- Switches atom ⇒ 0 to character

Now consider C_n rotations...

eg. NO_3^- (D_{3h})



Because the rotated basis vectors (x' and y') can be written as non-trivial linear combinations of the original basis vectors (x and y), the above rules fail.

∴ we must work out matrix representatives

$$x' = -\sin 30^\circ x - \cos 30^\circ y + 0z = -\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y + 0z$$

$$y' = \cos 30^\circ x - \sin 30^\circ y + 0z = \tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y + 0z$$

$$z' = 0x + 0y + z$$

or

$$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}$$

χ = sum of diagonal elements = 0

(and vectors on the oxygens also give 0)

Q. What is $\chi(\hat{S}_3)$?