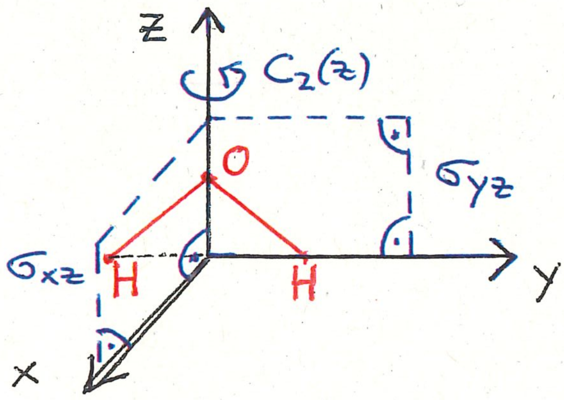
Symmetrieoperationen H_2O (in y-z-Ebene)



Symmetrieoperationen $\{E, C_2, \sigma_{xz}, \sigma_{yz}\}$

ergibt $\mathcal{C}_{nv}$ mit n = 2, $\qquad \mathcal{G} = \mathcal{C}_{2v}$

Transformationsmatrizen des Ortsvektors

$$\mathbf{M}(\sigma_{xz})\,\vec{\mathbf{r}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \vec{\mathbf{r}}$$

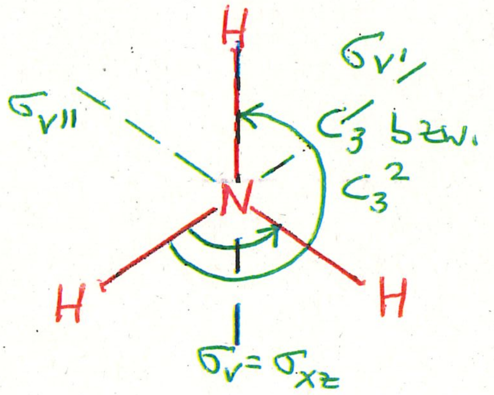
$$\mathbf{M}(\sigma_{yz})\,\vec{\mathbf{r}} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \vec{\mathbf{r}}$$

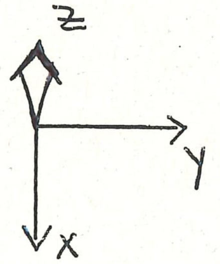
$$\mathbf{M}(\sigma_{xz})\mathbf{M}(\sigma_{yz}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \mathbf{M}(\sigma_{yz})\mathbf{M}(\sigma_{xz}) = \mathbf{M}(C_2(z))$$

und Kommutatorbeziehung $\Rightarrow$ $\mathcal{C}_{2v}$ ist abelsch

Symmetrien NH_3 (Draufsicht)





Symmetrieoperationen $\{E, C_3, C_3^2, \sigma_v, \sigma_{v'}, \sigma_{v''}\}$

ergibt $\mathcal{C}_{nv}$ mit $n = 3$, d.h. $\mathcal{C}_{3v}$

<u>Transformationsmatrizen des Ortsvektors</u>

$$\mathbf{M}(C_3)\,\vec{\mathbf{r}} = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \vec{\mathbf{r}}$$

$$\mathbf{M}(C_3)\mathbf{M}(\sigma_{xz}) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix} = \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\mathbf{M}(\sigma_{xz})\mathbf{M}(C_3) = \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix} \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$\neq \mathbf{M}(C_3)\mathbf{M}(\sigma_{xz})$ <u>nicht abelsch</u>

<u>Andere Fälle $(2 \neq n \neq 3)$</u>:

$$\sigma_v \sigma_{v'} = C(2(\beta-\alpha)) \; ; \quad \sigma_{v'} \sigma_v = C(2(\alpha-\beta))$$

$$C(2(\alpha-\beta)) = C(2(\beta-\alpha)) \iff 2 \cdot 2(\alpha-\beta) = 2\pi n$$

d.h. $\alpha - \beta = n\pi/2$ (nur $n=1$ sinnvoll)