

# Simetria e Orbitais Moleculares

## Aula zero

### Operações de simetria



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# Bibliografia

# Bibliografía básica - Simetria

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# Bibliografia – Simetria e Espectroscopia

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- TSUKERBLAT, B. S. *Group Theory in Chemistry and Spectroscopy. A Simple Guide to Advanced Usage*, Academic Press: Londres, 1994

# Bibliografia – Simetria e Química Inorgânica

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- PFENNIG, B. W. Principles of Inorganic Chemistry, John Wiley & Sons, Inc.: Hoboken, NJ, 2015.
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# Bibliografia – Referências adicionais

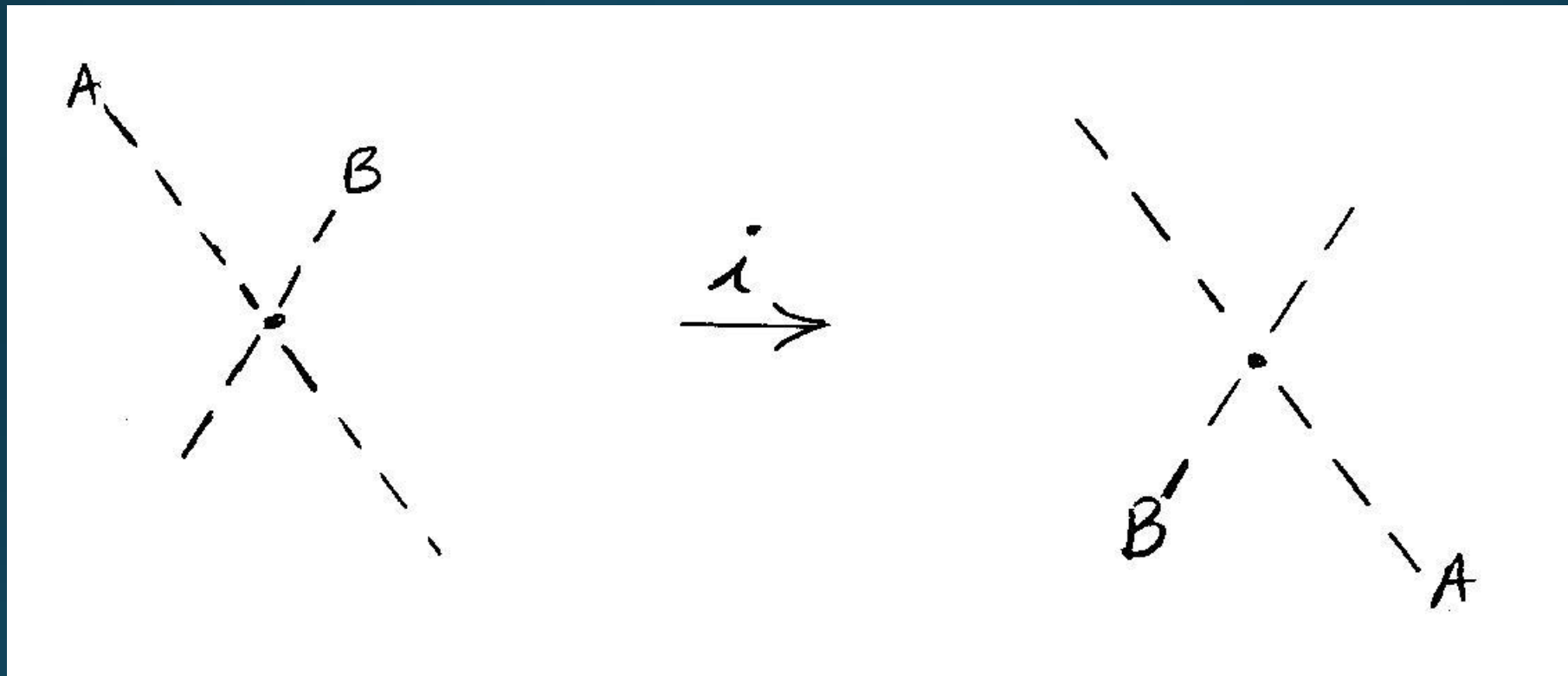
- BAIBICH, I. M.; BUTLER, I. S. A brief introduction to molecular orbital theory of simple polyatomic molecules for undergraduate chemistry students, *Quim. Nova* 35(7):1474-1476(2012).
- GRUSHOW, A. Is It Time To Retire the Hybrid Atomic Orbital? *J. Chem. Educ.* 88:860-862 (2011).
- LAING, M. No Rabbit Ears on Water. The Structure of the Water Molecule: What Should We Tell the Students. *J. Chem. Educ.* 64:124-128 (1987).

# Operações de Simetria

- operação identidade,  $E$
- operação centro de inversão,  $i$
- operação rotação,  $C_n$
- operação plano de reflexão,  $\sigma$
- operação rotação imprópria,  $S_n$

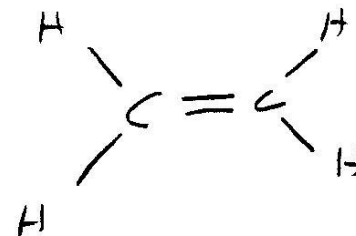
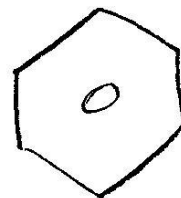
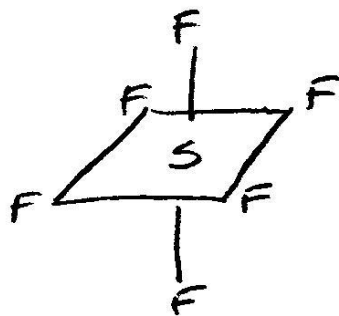
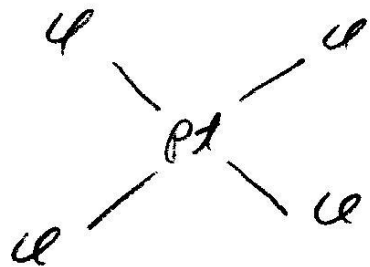


# Centro de inversão

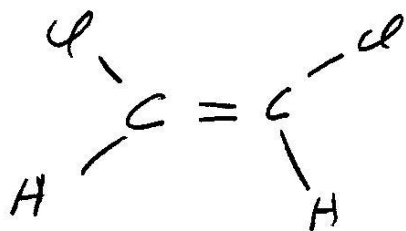
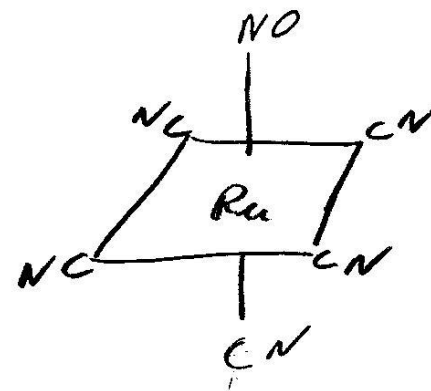
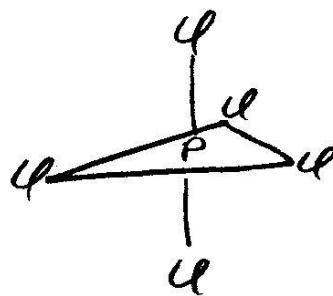
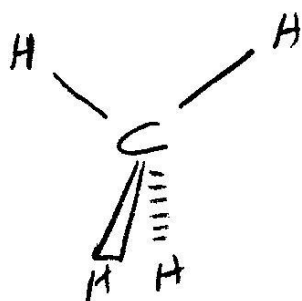
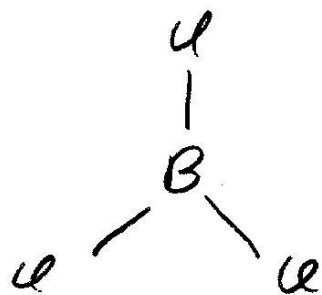


# Centro de inversão

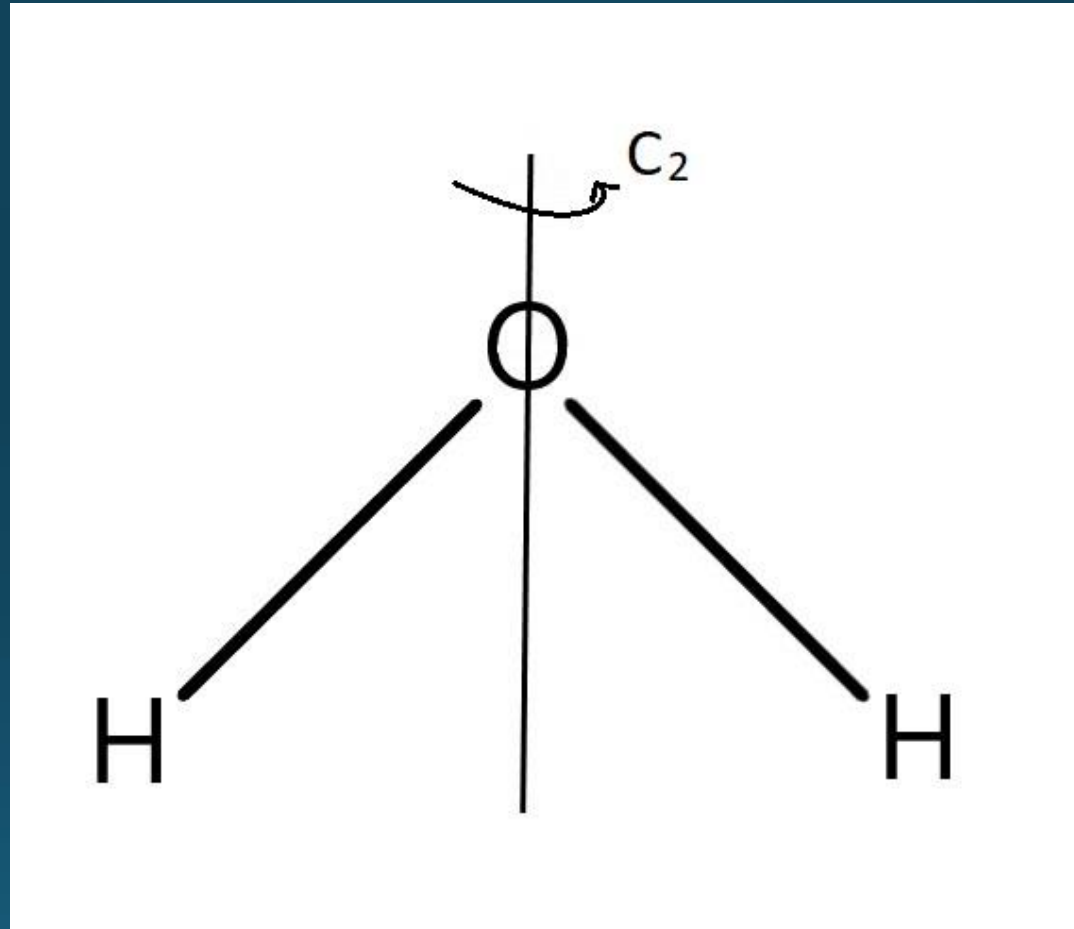
a)



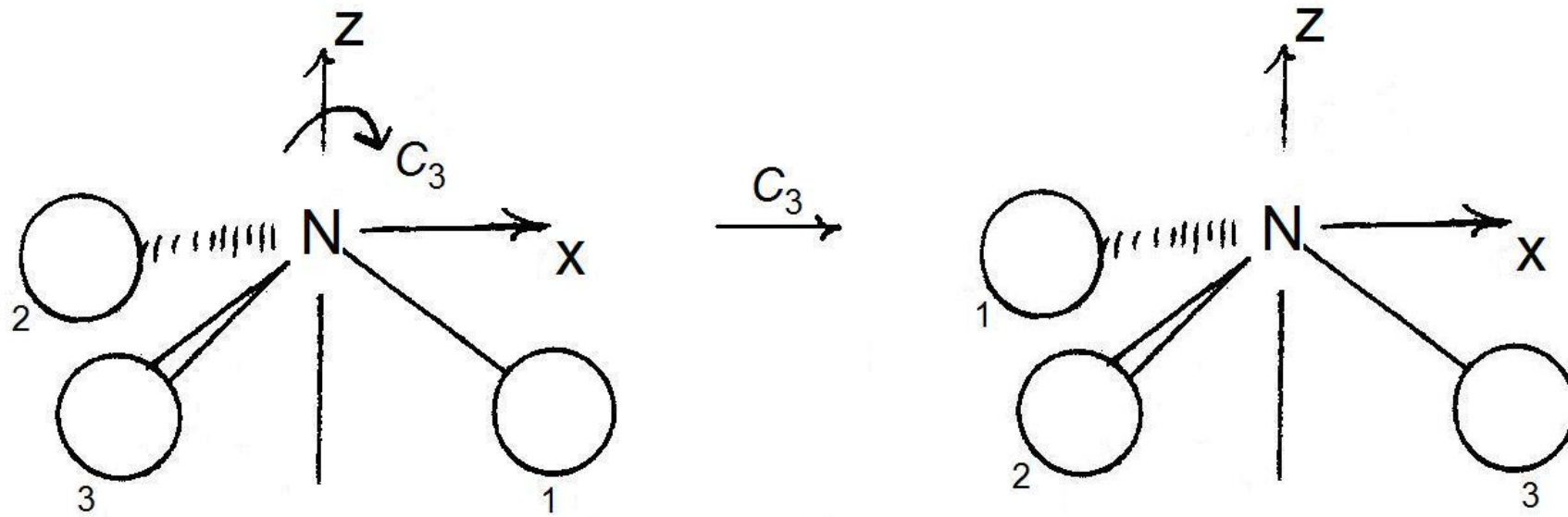
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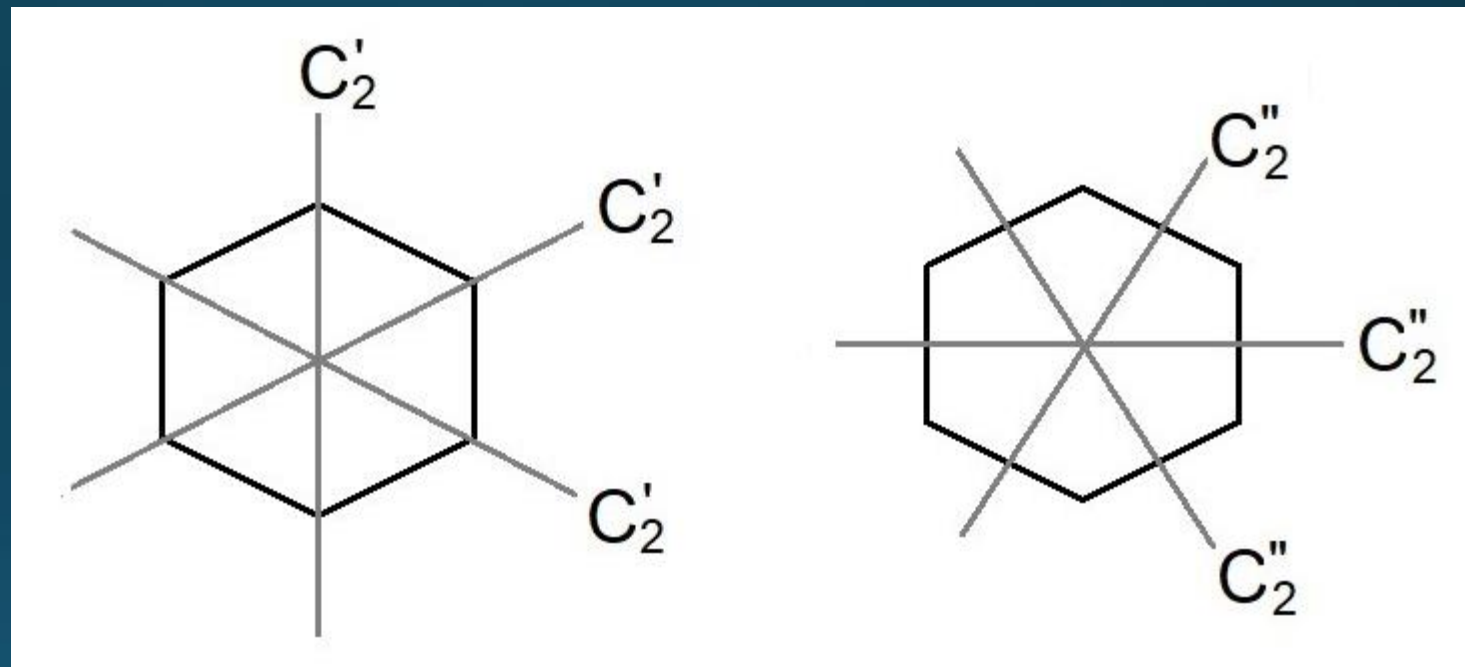
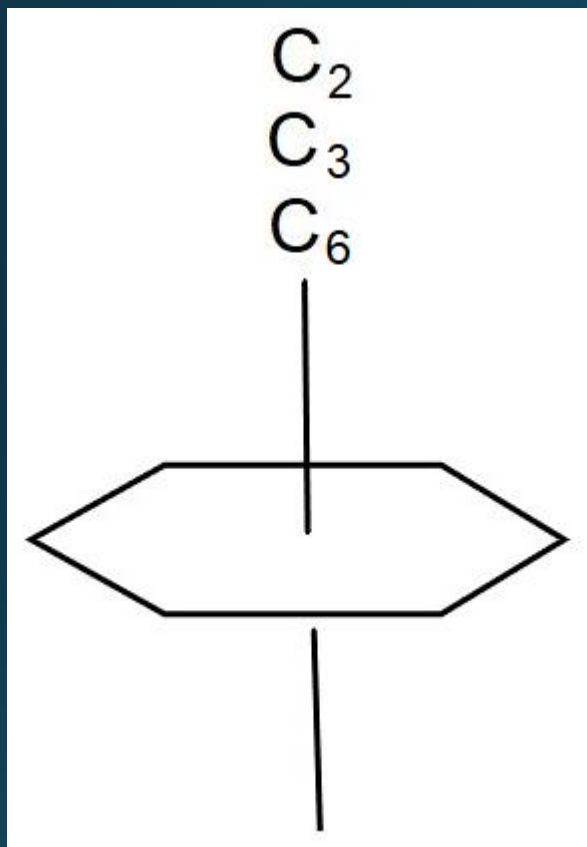
# Eixo de rotação



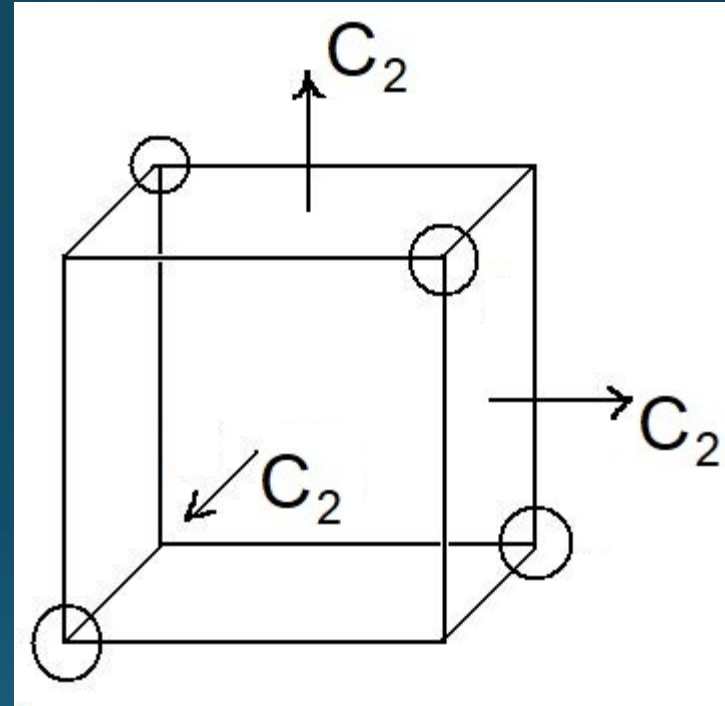
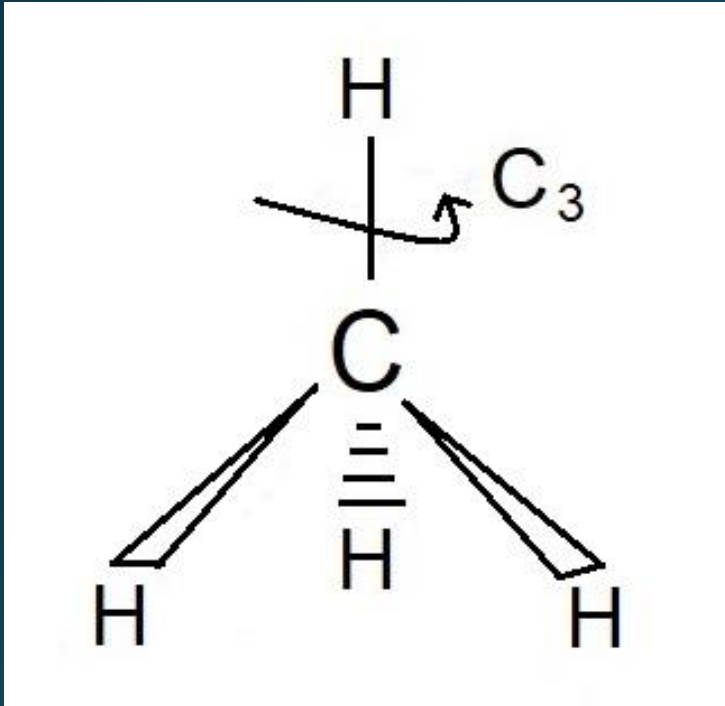
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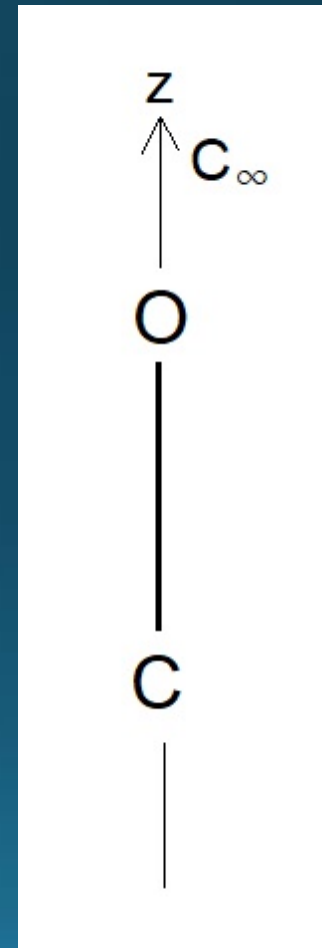
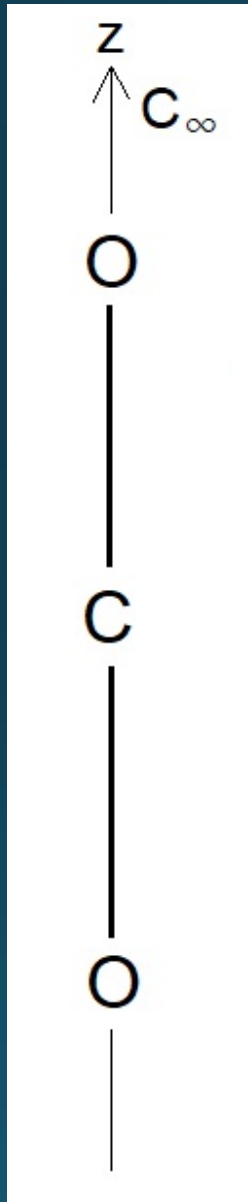
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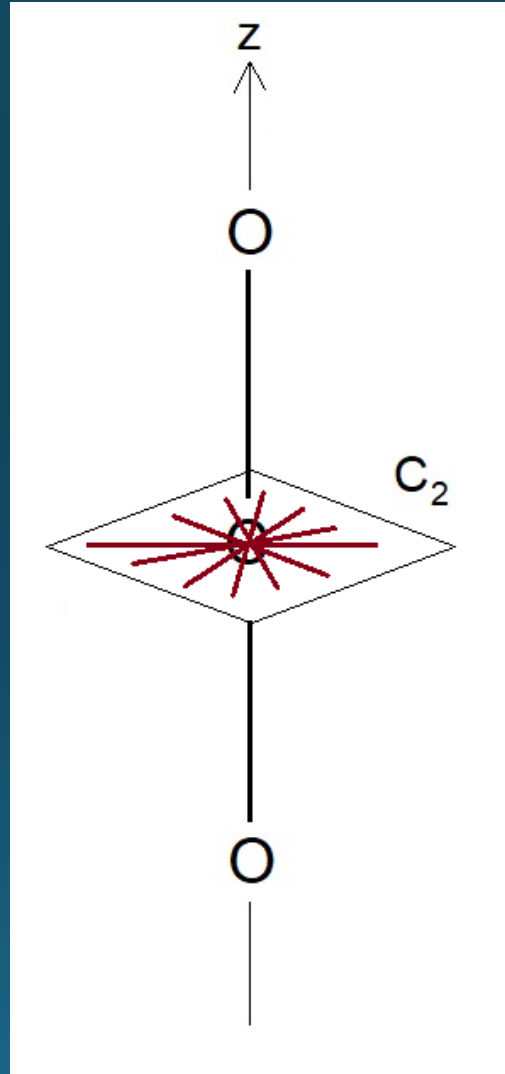
# Eixo de rotação



# Eixo de rotação - $C_\infty$

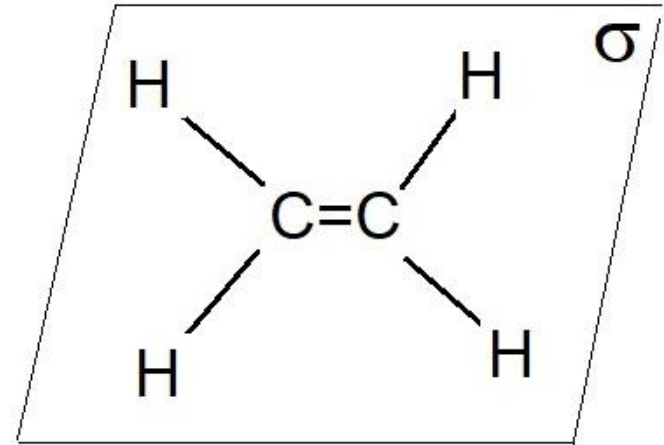
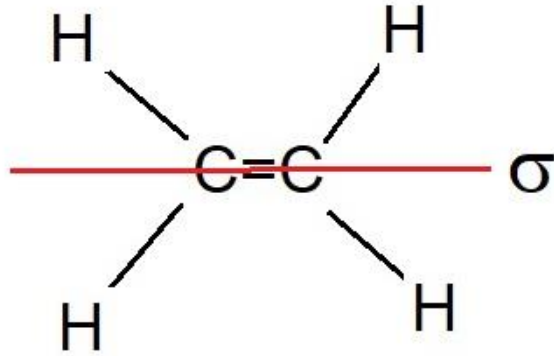
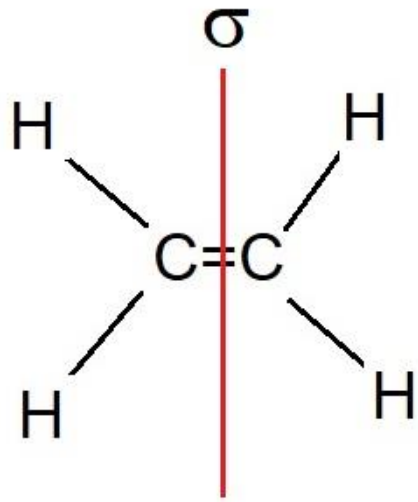


# Eixo de rotação

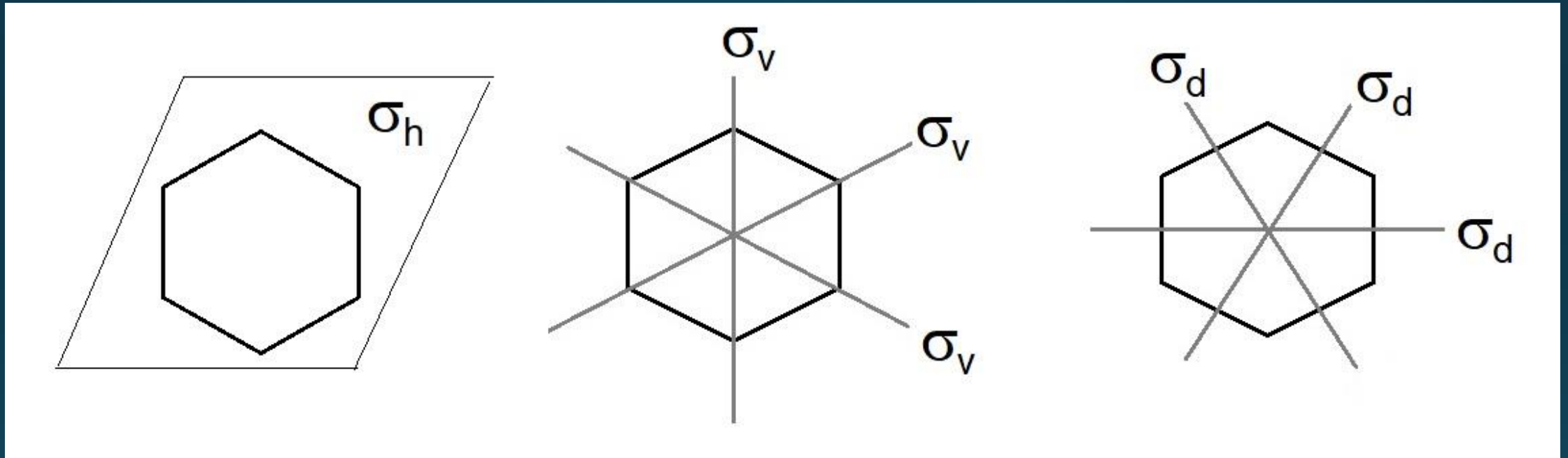




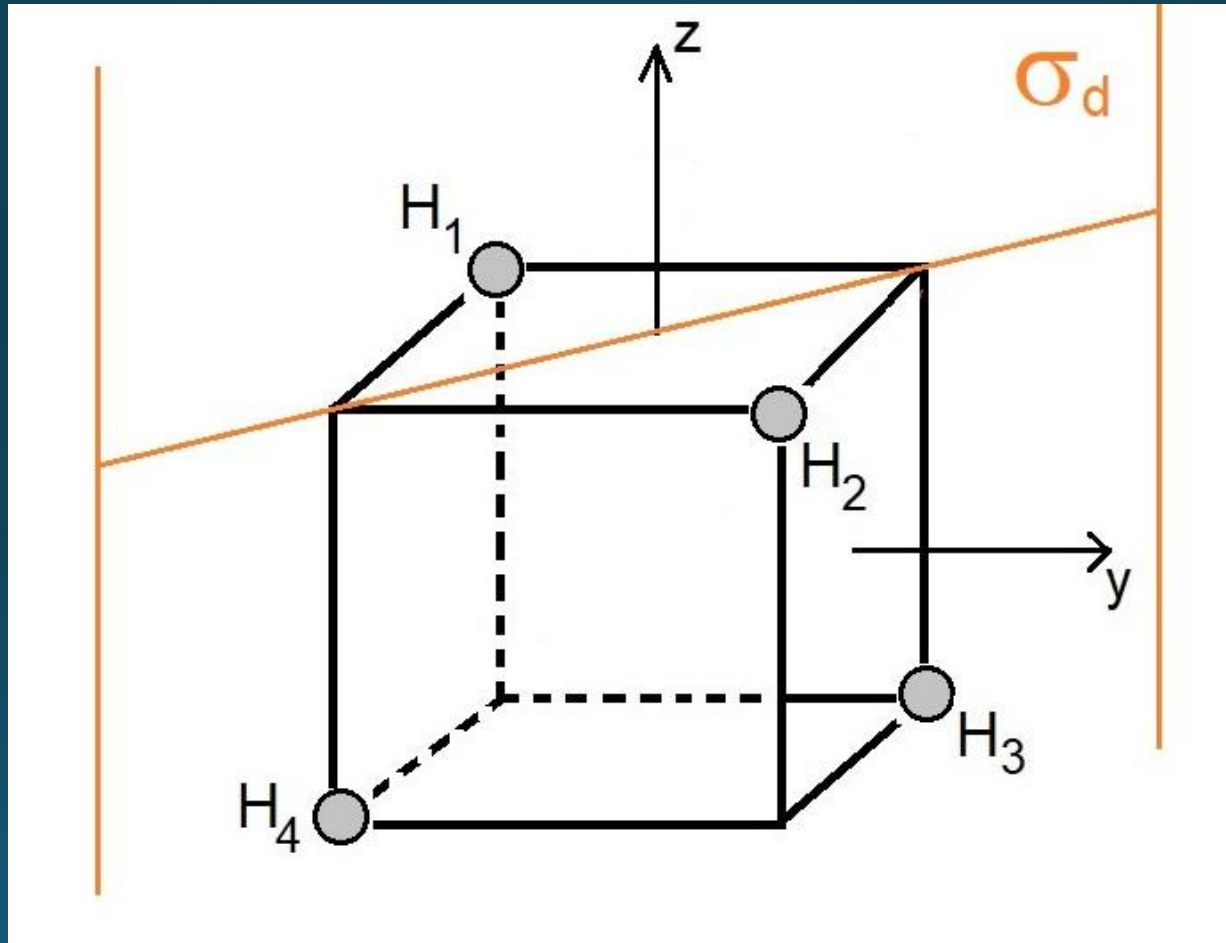
# Plano de reflexão ( $\sigma$ $\sigma_v$ $\sigma_d$ $\sigma_h$ )



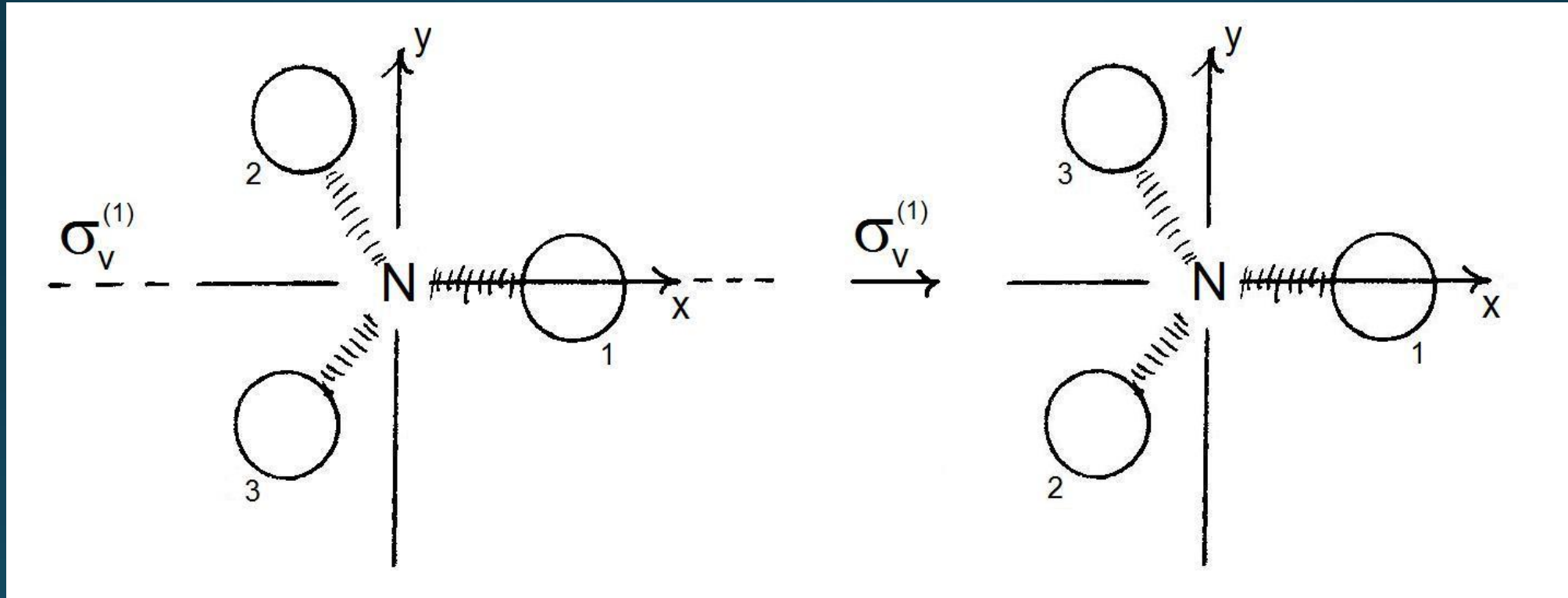
# Plano de reflexão ( $\sigma$ $\sigma_v$ $\sigma_d$ $\sigma_h$ )



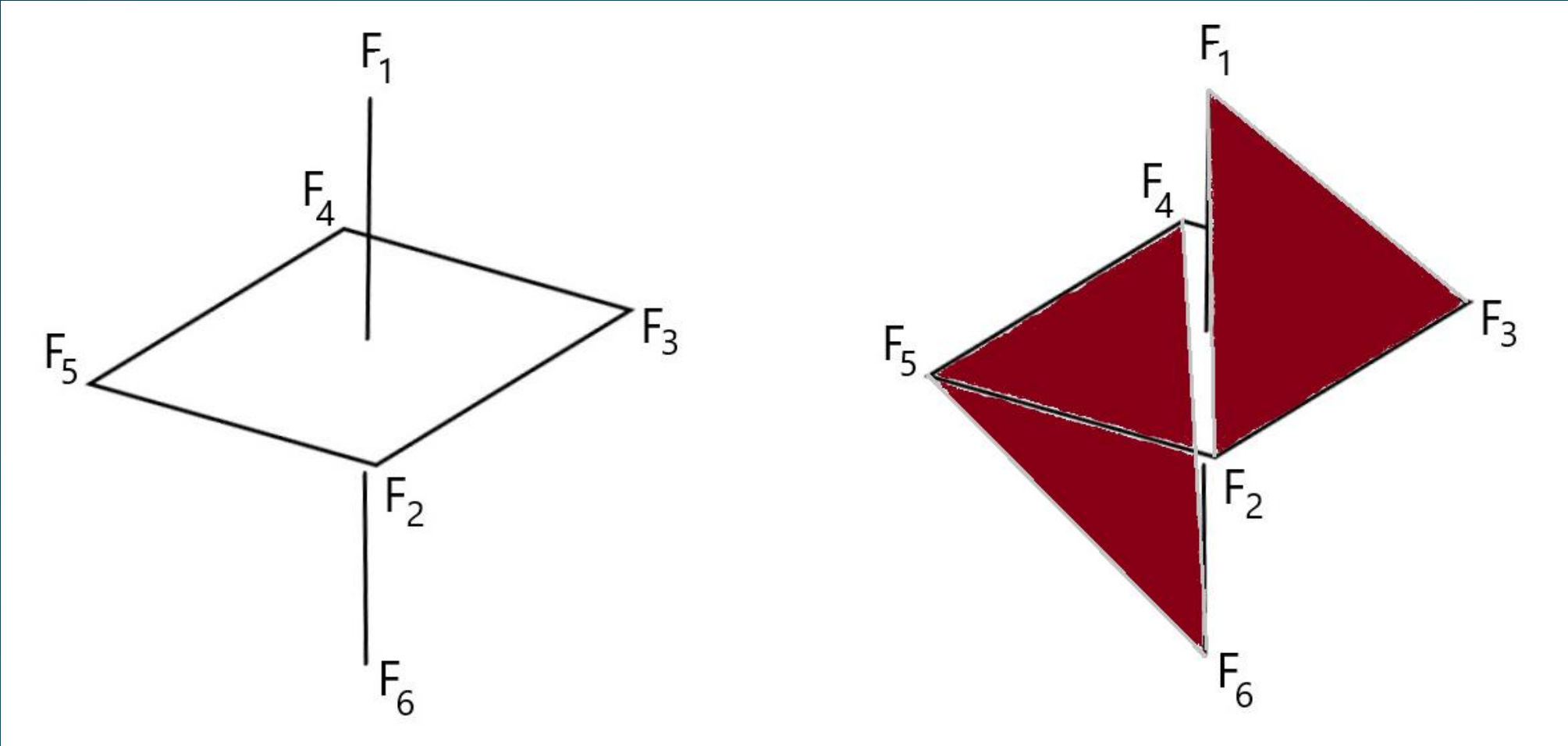
# Plano de reflexão ( $\sigma$ $\sigma_v$ $\sigma_d$ $\sigma_h$ )



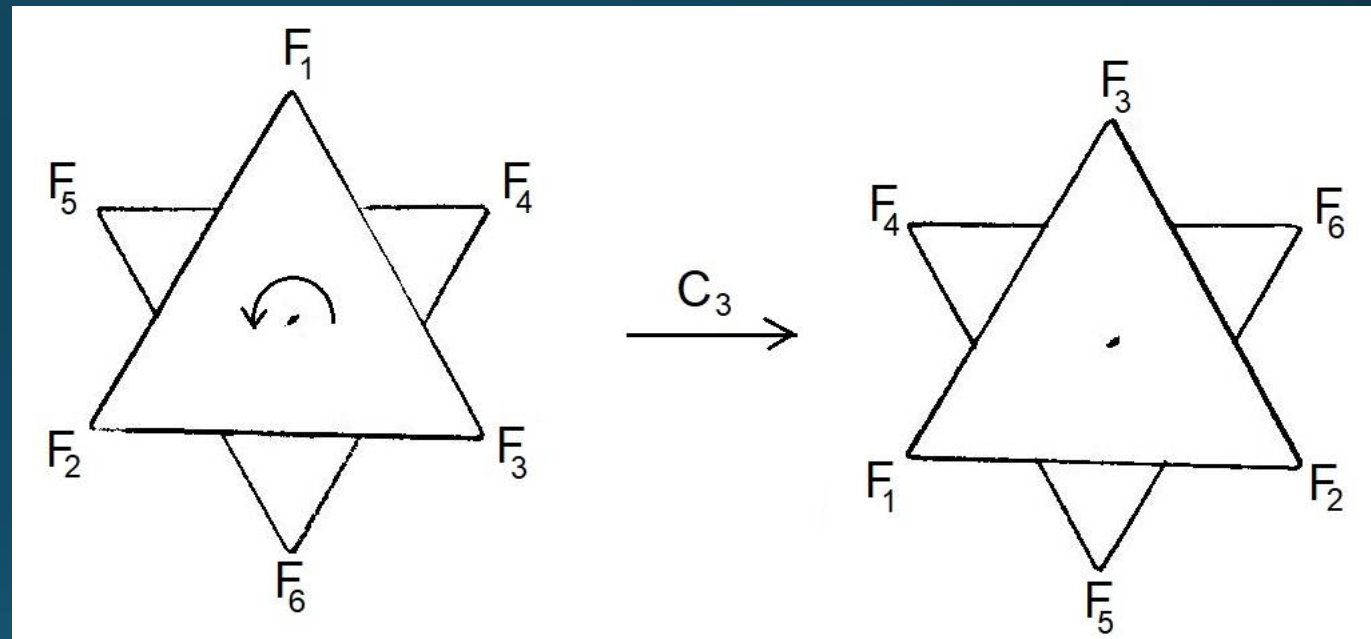
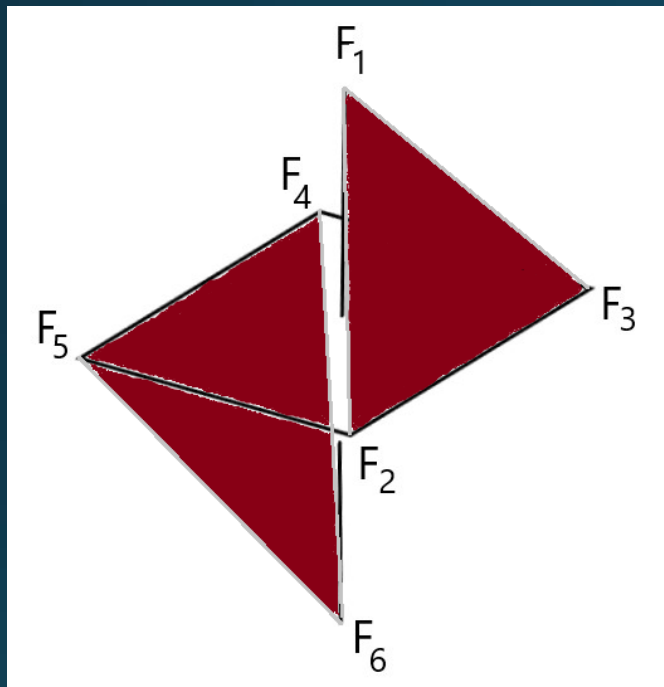
# Plano de reflexão ( $\sigma$ $\sigma_v$ $\sigma_d$ $\sigma_h$ )



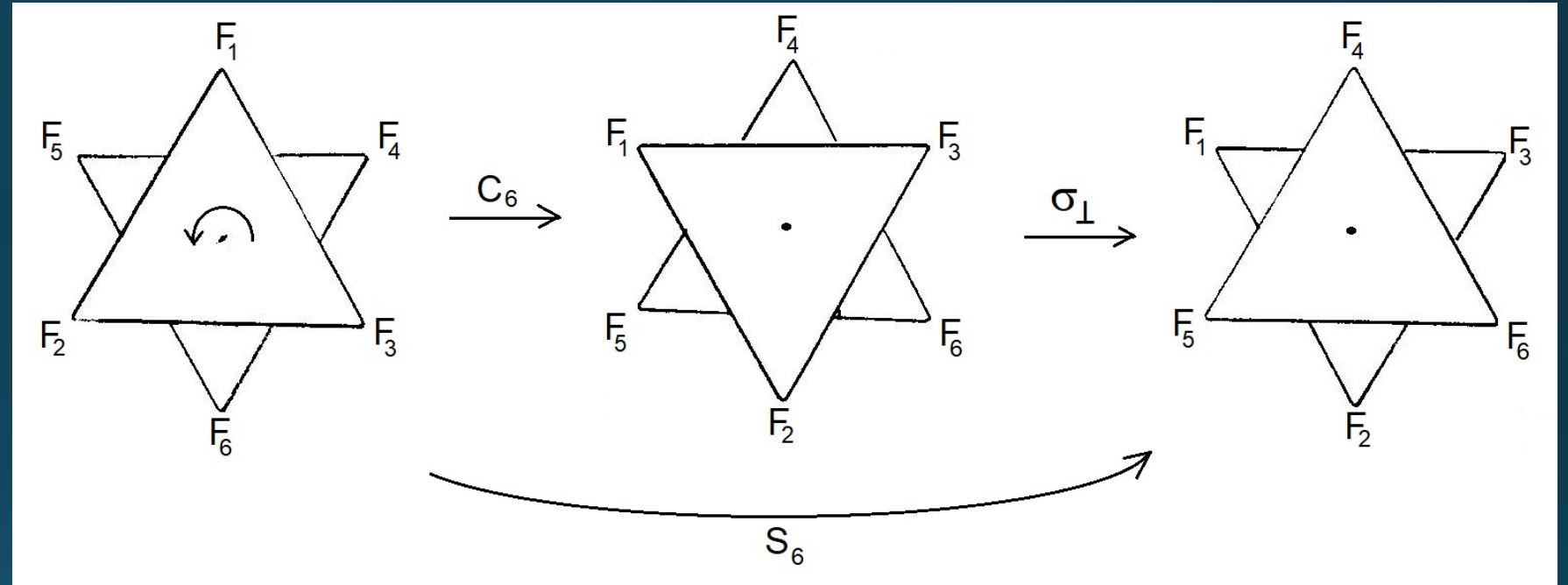
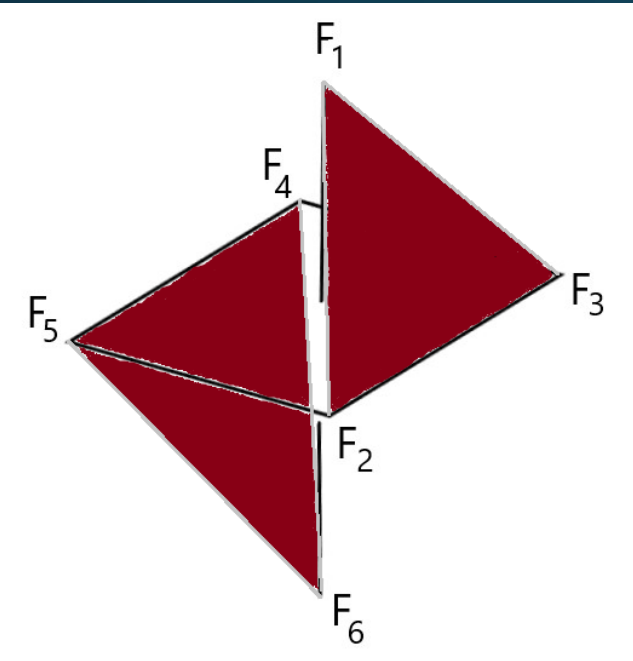
# Rotação imprópria



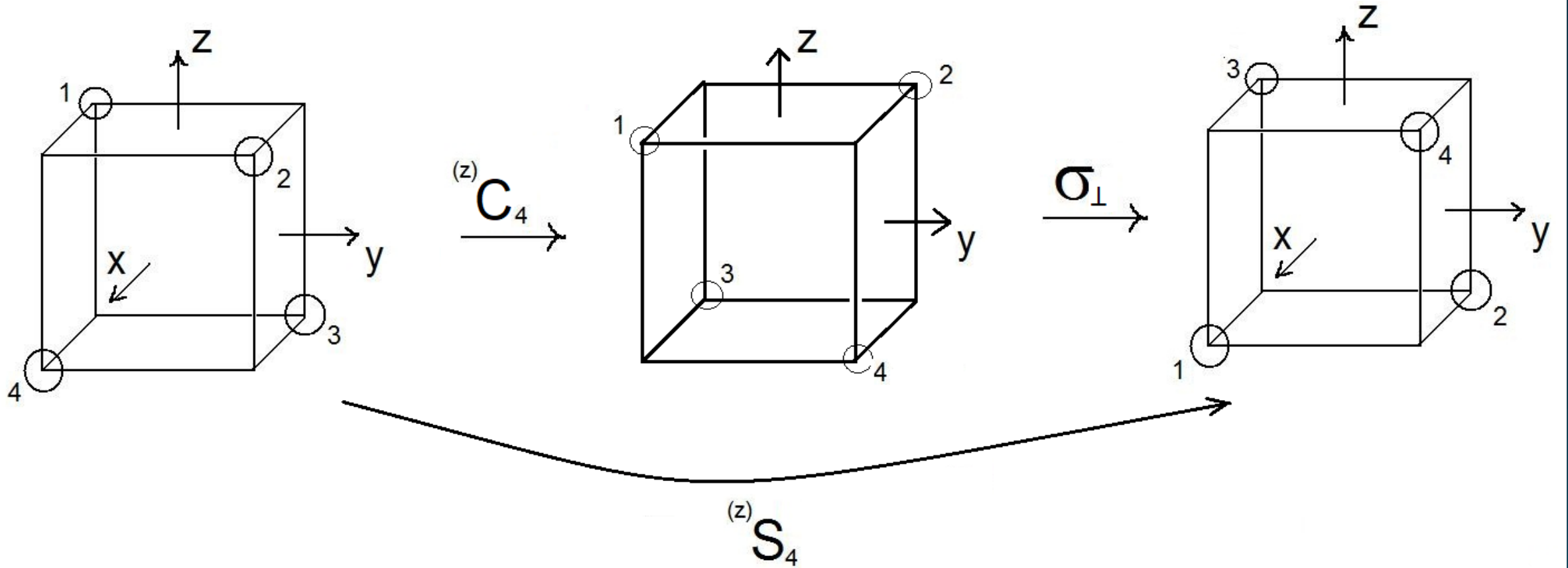
# Rotação $C_3$



# Rotação imprópria $S_6$



# Rotação imprópria $S_4$





$$C_1 = E$$

$$C_2 \quad C_2^2 = E$$

$$C_3 \quad C_3^2 = C_3^{-1} \quad C_3^3 = E$$

$$C_4 \quad C_4^2 = C_2 \quad C_4^3 = C_4^{-1} \quad C_4^4 = E$$

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$$S_1 = C_1 + \sigma = E + \sigma = \sigma$$

$$S_2 = C_2 + \sigma = i$$

$$S_3 = C_3 + \sigma$$

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$$S_3 = C_3 + \sigma$$

$$S_3^2 = C_3 + \sigma + C_3 + \sigma = C_3^2$$

$$S_3^3 = C_3 + \sigma + C_3 + \sigma + C_3 + \sigma = C_3^3 + \sigma = \\ = E + \sigma = \sigma$$

$$S_3^4 = 4 \times C_3 + 4 \times \sigma = C_3$$

$$S_3^5 = S_3^{-1} \text{ (não tem como simplificar)}$$

$$S_3^6 = 6 \times C_3 + 6 \times \sigma = E$$

# Atividade óptica

- Não apresentam atividade óptica as moléculas ou íons que possuam qualquer eixo de rotação impróprio ( $S_n$ ).
- Significa também que a presença de um plano de reflexão ( $S_1 = \sigma$ ) ou centro de inversão ( $S_2 = i$ ) não permite que uma molécula ou íon apresente atividade óptica, além de qualquer outro  $S_n$ .