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Fundamentals of Molecular Symmetry ***Exercises***

Week 3/11

3.1 Consider the group

$$\boldsymbol{C}_3(\mathrm{M}) = \{E, (123), (132)\}.$$

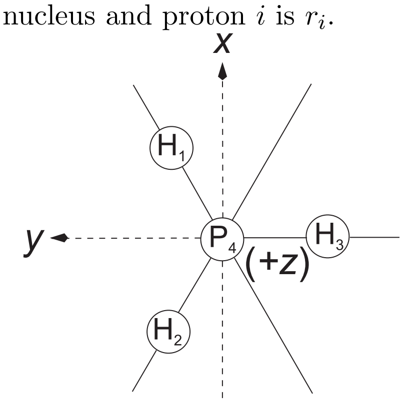
a) Determine the multiplication table, the class structure, and the characters of the irreducible representations of this group.

b) Consider a coordinate q_{A_1} with A_1 symmetry in $\boldsymbol{S}_3 = \{E, (123), (132), (12), (23), (31)\}$, a coordinate q_{A_2} with A_2 symmetry in $\boldsymbol{S}_3$ and a coordinate pair (q_a, q_b) with E symmetry in $\boldsymbol{S}_3$. Which representations of $\boldsymbol{C}_3(\mathrm{M})$ do these coordinates generate?

3.2 Consider the molecule PH_3 with the CNP group

$$\boldsymbol{S}_3 = \{E, (123), (132), (12), (23), (13)\}.$$

The three protons are labeled by $i = 1, 2, 3$. The internuclear distance between the P nucleus and proton i is r_i.



a) Determine the (reducible) representation of $\boldsymbol{S}_3$ that is generated by r_1, r_2 and r_3.

b) Calculate the characters of the reducible representation and complete the following character table

	E	(123)	(132)	(12)	(23)	(13)
Γ_{red}						

c) Use the matrix $\mathbf{V}$ to carry out similarity transformations for the matrices determined under a):

$$\mathbf{V} = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} & 0 \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} \end{pmatrix}.$$

You obtain a block diagonal representation. From the block diagonal matrices you can now 'isolate' two further representations. These are irreducible.

d) Add to the table from b) the characters of the two irreducible representations Γ_1 und Γ_2 from c).

e) Are the irreducible representations Γ_1 und Γ_2 homomorphic or isomorphic to $\boldsymbol{S}_3$?

Hint: The 3×3 matrices to be manipulated in Problem 3.2 are all *orthogonal*. If you do not know how an orthogonal matrix is defined, you can find the definition in the internet. For an orthogonal matrix $\mathbf{U}$,

$$\mathbf{U}^{-1} = \mathbf{U}^{\mathrm{T}}$$

where the superscript denotes transposition. Thus, orthogonal matrices can be easily inverted and that saves work by the solution of Problem 3.2.