University of Regensburg — Summer Term 2013

Applications of Group Theory

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Lectures	9.2.01, Mondays, 14:15
Exercises	7.1.21, Fridays, 10:15

Sheet 4

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1. Character of a class

The character of a matrix representative for a group element is nothing else that the trace of that matrix. The character is in reality associated to a class of symmetry operations thanks to the invariance of the trace under similarity transformations. Prove the latter statement.

2. Second orthogonality theorem for characters

Prove that the summation over all irreducible representations Γ_j yields

$$\sum_{\Gamma_j} \chi^{\Gamma_j}(\mathcal{C}_k) \left[\chi^{\Gamma_j}(\mathcal{C}_{k'})\right]^* = \frac{h}{N_k}\delta_{kk'}$$

where h is the order of the group and N_k is the order of the class $\mathcal{C}_k$. Hint: Start from the first orthogonality theorem and proof the unitarity of the matrix Q whose elements are defined as $Q_{ik} = \sqrt{\frac{N_k}{h}}\chi^{\Gamma_i}(\mathcal{C}_k)$. As a consequence of the second orthogonality theorem for characters derive the relation $\sum_i l_i^2 = h$ where the sum extends to all irreducible representations and l_i is the dimensionality of the i-th irreducible representation.

3. Reduce a representation

Suppose that you have the following set of characters: $\chi(E) = 4$, $\chi(\sigma_h) = 2$, $\chi(C_3) = 1$, $\chi(S_3) = -1$, $\chi(C_2') = 0$, $\chi(\sigma_v) = 0$.

1. Do these characters correspond to a representation of the point group D_{3h}? Is it irreducible? Justify your answers without invoking tabulated character tables.
2. If the representation is reducible, find the irreducible representations contained therein.
3. Give an example of molecule with D_{3h} symmetry.

Frohes Schaffen!