

Notes of **Advanced Physical Chemistry II**

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Introduction

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12 Group Theory: the Exploitation of Symmetry

Matrices

$\det(\mathbf{A}) = 0 \Rightarrow \mathbf{A}$ is a singular matrix.

12.1 The Exploitation of the Symm of a Mol Can Be Used to Significantly Simplify Numerical Calculations

12.2 The Symm of Mols Can Be Described by a Set of Symm Elements

E	
C_n	Rotation by $360^\circ/n$
σ	
i	
S_n	

Table 1: Symmetry elements and operators

Identity

Rotation

σ_h	horizontal
σ_v	vertical
σ_d	diagonal (vertical and bisects the angle between C_2 axis)

Table 2

Reflection

Inversion

Rotation Reflection

$$\hat{S}_n = \hat{\sigma}_h \times \hat{C}_n \quad (12.1)$$

12.3 Point Groups of Interest to Chemists

C_{nv}	Rotation by $360^\circ/n$
C_{nh}	
D_{nh}	
D_{nv}	
D_{nd}	
T_d	

Table 3: Symmetry elements and operators