

# 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 $360^\circ/n$
$\sigma$	
$i$	
$S_n$	

Table 1: Symmetry elements and operators

### Identity

### Rotation

$\sigma_h$	horizontal
$\sigma_v$	vertical
$\sigma_d$	diagonal (vertical and bisects the angle between $C_2$ axis)

Table 2

### Reflection

### Inversion

### Rotation Reflection

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

### 12.2.1 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

## 12.3 The Symm Operators of a Mol Form a Group

A set of operators form a group if they satisfy:

1. closed under multiplication 乘法封闭
2. associative multiplication 乘法结合律
3. only one identity operator 单位元
4. everyone has only one inverse 逆元

### 12.3.1 Point Group for Some Mols

No Symm Axis

$C_1$  – nothing

$C_s$  –  $\sigma$

$C_i$  –  $i$

$C_n$

$S_n$

$C_{nv}$  –  $C_n$  and  $n\sigma_v$

$C_{nh}$  –  $C_n$  and  $\sigma_h$

$D_n$  –  $C_n$  and  $nC_2 \perp C_n$

e.g. 一点点交错的  $C_3H_6$ ,  $C_2$  在 3 个角平分线处

$D_{nd}$  –  $C_n$ (also  $S_{2n}$ ) and  $nC_2 \perp C_n$  and  $n\sigma_d$

$D_{nh}$  –  $C_n$  and  $nC_2 \perp C_n$  and  $\sigma_h$

$T_d$  主轴是  $S_4$

$O_h$

$I_h$