

Notes of **Advanced Physical Chemistry II**

hebrewsnabla

September 4, 2019

Contents

12	Group Theory: the Exploitation of Symmetry	2
12.1	The Exploitation of the Symm of a Mol Can Be Used to Significantly Simplify Numerical Calculations	2
12.2	The Symm of Mols Can Be Described by a Set of Symm Elements	2
	Identity	2
	Rotation	2
	Reflection	2
	Inversion	2
	Rotation Reflection	2
12.2.1	Point Groups of Interest to Chemists	3
12.3	The Symm Operators of a Mol Form a Group	3
12.3.1	Point Group for Some Mols	3
	No Symm Axis	3
	C_n	3
	S_n	3
	C_{nv}	3
	C_{nh}	3
	D_n	3
	D_{nd}	3
	D_{nh}	3
	T_d	3
	O_h	3
	I_h	4

Introduction

TA: 刘琼 G403

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

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

12.2.1 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 – σ

C_i – i

C_n

S_n

C_{nv} – C_n and $n\sigma_v$

C_{nh} – C_n and σ_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 σ_h

T_d 主轴是 S_4

O_h

I_h

12.4 Symm Operators Can Be Represented by Matrices