

## Symmetry in Chemistry, Physics and Materials Science

### 0. Introduction

*(X.X: References to examples discussed during the course)*

#### 0.1. Motivation

- Symmetry: simplified description of geometry

⇒ Simplified description (“rules”) for

1. electronic structure
2. physical properties
3. spectroscopy
4. reactivity

This course: molecules, surfaces, solids (crystals)

(everything by simple considerations, no extensive calculations)

#### 0.2 Outline

1. Symmetry of molecules

*(0.1: C<sub>60</sub> molecule)*

2. Symmetry of surfaces and solids

*(0.2: Pt/Pt(110), STM)*

3. “Compact course” group theory

4. Group theory and quantum mechanics

5. Organic chemistry:

electronic structure and reactions

*(0.3: Symmetry elements in coronene)*

6. Anorganic chemistry:

ligand-field theory and spectroscopy

*(0.4: JT effect in octahedral complex)*

7. Spectroscopy:

normal vibrational modes and spectroscopy

*(0.5: Exclusion rule in vibrational spectroscopy)*

8. Crystal physics:

Physical properties of crystals, description by tensors

*(0.6: Double diffraction in calcite)*

9. Electronic structure of solids:

electronic and vibrational band structures

*(0.7: Fermi surface of Cu)*

03. Literature

- F. A. Cotton: “Chemical Applications of Group Theory”, John Wiley & Sons, 1990.  
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- B. S. Wherrett: “Group Theory for Atoms, Molecules and Solids”, Prentice Hall International, 1986 (\*\*\*)
- G. Burns: “Introduction to Group Theory with Applications”, Academic Press, 1977.
- W. Ludwig, C. Falter: “Symmetries in Physics”, Springer, 1988.
- M. Lax: “Symmetry Principles in Solid State and Molecular Physics”, John Wiley & Sons, 1974.
- M. F. C. Ladd, “Symmetry in Molecules and Crystals”, John Wiley & Sons, 1989.
- G. Davidson: “Introductory Group Theory for Chemists”, Elsevier Publishing, 1971.
- D. Steinborn: “Symmetrie und Struktur in der Chemie”, VCH, 1993.
- K. Mathiak, P. Stingl : “Gruppentheorie”, Akademische Verlagsgesellschaft, 1968.

special topics:

Group theory and quantum mechanics:

- P. W. Atkins: “Molecular Quantum Mechanics”, Oxford University Press, 1989.

Molecular vibrational spectroscopy:

- E. B. Wilson, Jr., J. C. Decius, P. C. Cross: “Molecular Vibrations”, Dover Publications, 1955.

Group theory and crystal physics:

- E. Hartmann: “An Introduction to Crystal Physics”, International Union of Crystallography, 2001 (free download at: [www.iucr.org](http://www.iucr.org))
- J. F. Nye: “Physical Properties of Crystals”, Oxford University Press, 2000.
- S. Haussühl: “Kristallphysik”, Physik-Verlag / VCH 1983.

Electronic structure of solids:

- S. L. Altmann: “Band Theory of Solids: An Introduction from the Point of View of Symmetry”

#### 04. Supporting information

Lecture notes and supporting information will be made available for download at

[www.imprs-cs.mpg.de](http://www.imprs-cs.mpg.de)

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