QMC1808 – Group Theory and Molecular Point Groups

Syllabus

UNIT 1 - ELEMENTS OF SYMMETRY AND OPERATIONS

1.1 - Concept of symmetry

1.2 - Elements of symmetry and operations: Generalities; Proper rotation axis *(C*p); Mirror plane*(s);* Inversion Center*(i);* Improper rotation axis *(S*p)

1.3 - The Cartesian coordinate system

UNIT 2 - POINT GROUP THEORY

2.1 - General group properties: Application of group axioms in point groups; Multiplication tables; Cyclic point groups; Symmetry classes

UNIT 3 - SYSTEMATICS OF MOLECULAR POINT GROUPS.

3.1 - Symbology

3.2 - Type I - Non-axial groups

3.3 - Type II - Groups *C*

3.4 - Type III - Groups *D*

3.5 - Type IV - Polyhedral groups

3.6 - Type V - Rotational groups

3.7 – Subgroups and supergroups

3.8 - Organization chart for molecular point symmetry classification

UNIT 4 - CHARACTER CHART

4.1 - Vector representation of degrees of freedom: Definition of degree of freedom; Vector representation

4.2 - Angular molecule - AB2: Translation vectors; Rotational vectors; Vibrational vectors; Character table construction; Character table laws

4.3 - Pyramidal molecule - AB4

4.4 - Mulliken Symbology

4.5 - General form for translation and rotation characters: Axial rotation of a point; Proper rotation axis *(C*p); Inversion Center *(i);* Mirroring plane *(s);* Improper rotation axis *(S*p)

4.6 - Vibrational activity: Vibrational modes active in infrared; Active vibrational modes in Raman; Exclusion principle.

UNIT 5 - VIBRATIONAL ANALYSIS

5.1 - Formalism of the representation of the sum of the degrees of molecular freedom

5.2 - Reduction formalism with correlation between degree of freedom and kind of symmetry

5.3 - Internal coordinates of a molecule

5.4 - Vibrational spectrum of molecule AB3 - active vibrational modes in infrared and Raman: AB3 molecule with pyramidal symmetry; AB3 molecule with trigonal-planar symmetry

5.5 - Vibrational spectrum of molecule AB2 - active vibrational modes in infrared and Raman: Angled AB2 molecule; Linear AB2 molecules

5.6 - Active Raman and IR vibrational modes in the C≡O molecule coordinated in metal pentacarbonyl derivative

5.7 - Active Raman and IR vibrational modes in the molecule with regular octahedral symmetry

5.8 - Active Raman and IR vibrational modes in molecule with regular tetrahedral symmetry

5.9 - Active vibrational modes in reducing symmetry in the molecule with polyhedric symmetry *T*d and *O*h

UNIT 6 - INFRARED SPECTRA OF METAL CARBONILES

6.1 - Metallic carbonyl with polyhedric symmetry *O*h and derivative thereof: Type $M(CO)_6$; Type $M(CO)_5X$; Type $M(CO)_4X_2$; Type $M(CO)_3X_3$; Type $M(CO)_2X_4$

6.2 - Metallic carbonyl with symmetry *D*3h and derived thereof: Type $M(CO)_5$; Type $M(CO)_4X$; Type $M(CO)_3X_2$

6.3 - Metallic carbonyl with symmetry *T*d and derived thereof: Type $M(CO)_4$; Type $M(CO)_3X$; Type $M(CO)_2X_2$

6.4 - Multinuclear metal carbonyls: Type $M_2(CO)_{10}$; Type $M_2(CO)_9$

6.5 - Active vibrational modes in correlation with the local symmetry of a metallic and derived carbonyl: Type $M_3(CO)_{12}$; Type η^5-$C_5H_5M(CO)_3X$; Type η^5-$C_5H_5M(CO)_3$

UNIT 7 - CORRELATION WITH CRYSTALLOGRAPHIC SYMMETRY

7.1 - Correlation of Hermann-Mauguin's symbology with Mulliken's symbology

7.2 - One-dimensional symmetry classes

7.3 - Symmetry elements and symmetrical equivalence operations in one-dimensional spatial networks and groups

7.4 - Symmetry elements and symmetrical equivalence operations in two-dimensional networks and spatial groups

7.5 - Symmetry elements and symmetrical equivalence operations in three-dimensional spatial networks and groups

7.6 - Crystalline symmetry - crystallographic point groups. Symbology of Schönflies

Bibliography

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HAHN, T.; **International Tables for Crystallography**, Vol. A, 5th Ed., The International Union of Crystallography/Springer, New York, 2005.

KUNZE, U.; LORENZ, I.-P.; **Gruppentheorie und Molekülsymmetrie** (authorized translation).

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Additional Bibliography

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