

COURSE SYLLABUS

1. Identification

Code and title: QUP 301 – Advanced Inorganic Chemistry

Professor: Maria do Carmo Martins Alves and Jackson Damiani Scholten

Level: Master and Doctorate

Credit hours: 3

Revised: August_2021

2. Summary

Molecular symmetry and group theory. Bonding theories in coordination compounds. Stability and thermodynamic aspects of coordination compounds.

3. Objective

Introduction to the concepts of symmetry and group theory as tools to study the chemical bonding in molecules and complexes of transition metals.

4. Contents

Definitions and theorems of group theory. Molecular symmetry and point groups. Group representations. Techniques and relationships for applications in chemistry. Formulation of hybrid orbitals. Calculation of the symmetry adapted orbitals with the use of the projection operator for sigma and pi bonding. Bonding theories in coordination compounds. Valence bond theory, crystal field theory, molecular orbital theory. Thermodynamic stability of coordination compounds.

5. Assessment

The evaluation will consist of two examinations and one seminar (S). The students with simple mean ($M = (E1 + E2) / 2$) below 6.0 must take a final examination (E3). The final grade (FG) will be calculated according to the equation: $FG = M \times 0.6 + S \times 0.4$. For students who take the final examination the final grade (FG) will be calculated according to the equation: Mean of the Final Proof (MPF) = $(M \times 0.4) + (E3 \times 0.6)$ and $FG = (MPF) \times 0.6 + S \times 0.4$. The student who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:

A: grade equal to or above 9.0

B: grade equal to or above 7.5 and below 9.0

C: grade equal to or above 5.0 and below 7.5

D: grade below 5

FF: lack of frequency

6. Methodology

Lectures, exercises lists, seminars and examinations.

7. Bibliography

- R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, Inc. 1998.

- F. A. Cotton, Chemical Applications of Group Theory. New York: Wiley Interscience, 1990.



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- G. L. Miessler, P. J. Fischer and D. A. Tarr, Inorganic Chemistry, 5th ed. Upper Saddle River: Pearson, 2014.
- D. J. Willock, Molecular Symmetry, John Wiley & Sons Ltd, Wiltshire, 2009.
- B. Douglas, D. Mc Daniel e J. Alexander, Concepts and Models of Inorganic Chemistry, 2ª Ed. New York: John Wiley & Sons, 1997.
- D. Shriver; P. Atkins and T. Overton, Inorganic Chemistry - Fourth Edition, Oxford, 2006.
- S. F. A. Kettle, Physical Inorganic Chemistry: A coordination chemistry approach. Oxford. Oxford University Press, 1998.
- R. S. Drago, Physical Methods in Chemistry, Saunders, 1977.
- I. S. Butler and J. F. Harrod, Inorganic Chemistry, Principles and Applications. USA: The Benjamin/Cummings Publishing Company, 1989.
- C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Harlow Pearson Education, 2008.
- D. A. McQuarrie and J. T. S Dimon, Physical Chemistry: A molecular approach, University Science Books, 1997.
- Selected publications in specialized scientific journals.