MÉTODOS MATEMÁTICOS I

Resume

This course develops the fundamental mathematical tools for post-graduated students who aim to focus on topics in theoretical and physical chemistry during their Ph.D. studies. The treated topics are: vectorial algebra, matrix algebra, coordinate transformations, group theory, molecular symmetry. During the course the students are faced with representative problems from theoretical and physical chemistry.

Contents

Vector Algebra

- Vector definition and vector operations
- Vector rules
- Scalar product, cross product, triple vectorial products
- Directional derivatives (gradients), divergence, curl, Laplacian
- Green's, divergence, curl and Stoke's theorems

Matrix Algebra

- Matrix definition and matrix operations
- Matrix rules
- Equation systems, including eigenvalue equations
- Definition of determinant
- Determinant rules
- Calculation of determinants

Coordinate Transformations

- Introduction to general curvilinear coordinate system
- Spherical coordinate system
- Cylindrical coordinate system

Group Theory

- Definitions of groups
- Mappings
- Binary operations
- Construction of a group
- Terminology of groups

Molecular Symmetry

- Symmetry elements and symmetry operations
- Point groups
- Classification of molecules into point groups
- Reducible and irreducible representation

Suggested basic literature

- Mathematical Methods in Physical Science, M.L. Boas, J. Wiley & Sons, 1983
- Matematik in der Chemie, K. Jug, Springer Verlag, 1993
- Symmetry and Spectroscopy, D.C. Harris, M.D. Bartolucci, Dover Publications Inc., 1978
- Group Theory and Chemistry, M.D. Bishop, Dover Publication Inc. , 1973