KARPAGAM ACADEMY OF HIGHER EDUCATION
(Deemed to be University)
Established Under Section 3 of UGC Act 1956)

Coimbatore – 641 021.

SYLLABUS

Semester-V

16CHU512B APPLICATIONS OF COMPUTERS IN CHEMISTRY PRATCTICAL 4H 2C

Instruction Hours/week: L:0 T:0 P:4 Marks: Internal: 40 External: 60 Total:100

Scope

The course deals with the Computer programs based on numerical methods for Roots of equations, Numerical differentiation, Numerical integration and matrix operations.

Objectives

This lab course enable the student to do experiments and to

1. Understand the basics of computers in chemistry
2. Understand to find the roots of equation
3. Understand the the numerical differentiation and integration
4. Understand matrix operations.

Methodology

Computer programmes

Computer programs based on numerical methods for

1. Roots of equations: (e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid).
2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
3. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.
4. Matrix operations. Application of Gauss-Siedel method in colourimetry.
5. Simple exercises using molecular visualization software.

Suggested Books:

1. McQuarrie, D. A. (2008). *Mathematics for Physical Chemistry*. University Science Books.
2. Mortimer, R. (2005). *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier.
3. Steiner, E. (1996). *The Chemical Maths Book* . Oxford University Press.
4. Yates, P. (2007). *Chemical Calculations.* 2nd Ed. CRC Press.
5. Harris, D. C. (2007). *Quantitative Chemical Analysis*. 6th Ed. Chapters 3-5. Freeman.
6. Levie, R. De. (2001). *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press 487 pages.
7. Noggle, J. H. (1985). *Physical Chemistry on a Microcomputer.* Little Brown & Co.
8. Venit, S.M. (1996). *Programming in BASIC: Problem solving with structure and style.* Delhi: Jaico Publishing House.
9. Riyazuddin .P (2012). *Computers in chemistry,* International Publishing House Pvt. Ltd.,

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DEPARTMENT OF CHEMISTRY

LECTURE PLAN

APPLICATION OF COMPUTERS IN CHEMISTRY-PRACTICAL

Name of the Faculty: B. Prabha
Department : CHEMISTRY
Semester V
Year : III
Course Code : 17CHU512B
Section : A & B

Total no. of hour's: 12 Hours

S.NO	Lecture Hours	EXPERIMENT TOPICS
1	4	Writing the experimental Procedure
2	4	Introduction to computer programs based on numerical methods
3	4	Roots of equation (Volume of Vander-Walls gas comparison with ideal gas)
4	4	Numerical differentiation (Potentiometric titration)
5	4	Viva-voce
6	4	Numerical Integration (entropy/enthalpy change from heat capacity data)
7	4	Probability distribution and means (gas kinetic theory)
8	4	Matrix Operations (Gauss-Siedel method in colourimetry)
9	4	Simple exercise using molecular visualization software
10	4	Viva-voce
11	4	Revision
12	4	Model Exam

Support Materials:

Text books : Riyazuddin P. (2012). *Computers in Chemistry, T.K International Publishing House Pvt. Ltd.,*