Republic of Iraq

The Ministry Of Higher Education

& Scientific Research

University: University of Baghdad
College: College of Science for Women
Department: Department of chemistry
Lecturer name: Shaimaa Rajab Baker
Qualification: MSc. Inorganic chemistry

Syllabus Form

Instructor Name	MunaSarhanSando
E-mail	munass @ csw.uoboghdad.edu
Course Title	Computational chemistry
Course Coordinator	Computer programs
Course Objectives	Enable students to learn more about computer hardware and software.
Course Description	Chem. Draw Ultra 10.0,(2006)
Textbook	• Computer Organization and Architecture: Designing for Performance, by William Sallings,23 May 2002. • Selected Topics About Computer Organization
References	• Computer Organization and Architecture: Designing for Performance, by William Sallings, 23 May 2002. • Selected Topics About Computer Organization

Course Assessments	Term Tests	Laboratory	Quizzes	Project	Final Exam
	As(25%)	As(5%)	As(5%)	As(5%)	As(60%)

General Notes	Type here general notes regarding the course

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Stage:

Lecturer name:

Qualification:

Place of work

Course Weekly Outline

Week	Date	Topes Covered	Lab. Experiment Assignments	Notes
1				
2				
3				
4				
5				
6				
7				
8				
9				
10				
11				
12				
13				
Half – year break				
17	22/2/2016		Quantum theory, Schrodinger equation, huckel theory Chem.Office(2006),chem.(3D) program(introduction)	

18	29/2/2016		Calculate theory, Abinitio, hartreefock method, Calculate internuclear distances of molecules	
19	7/3/2016		density functional theory, semi-empirical methods Calculate total energy of Molecules	
20	14/3/2016		Zero Differential overlap(ZDO), Calculate Z-Matrix of Molecules	
21	28/3/2016		Austin model 1(AM1), parameterize on 3 of MNDO(PM3) molecular Mechanic	
22	4/4/2016		Exam	
23	11/4/2016		modified neglect of Differential overlap(MNDO) Calculate IR-spectrum of molecules and found the chart.	
24	18/4/2016		Calculate the NMR spectrum and found the chart	
25	25/4/2016		Molecular modeling programs, Gaussiano3, chem. office (MOPAC) Found HOMO and LUMO of molecules	

26	2/5/2016		Exam	

Instructor Signature: **Dean Signature:**