



UNIVERSITAS NEGERI YOGYAKARTA
 FACULTY OF MATHEMATICS AND NATURAL SCIENCES
 DEPARTMENT OF CHEMISTRY
 1 Colombo Street Yogyakarta 55281
 Phone (0274) 565411, Ext. 1398, Fax (0274)548203
 Website: <http://kimia.fmipa.uny.ac.id>, E-mail: kimia@uny.ac.id

Bachelor of Science in Chemistry

MODULE HANDBOOK

Module name:	Quantum Chemistry						
Module level, if applicable:	Undergraduate						
Code:	KMA 6201						
Sub-heading, if applicable:	-						
Classes, if applicable:	2						
Semester:	5 th						
Module coordinator:	Dr. Suwardi						
Lecturer(s):	1. Dr. Suwardi 2. Dr. Crys Fajar Partana 3. Agus Salim, M.Si.						
Language:	Bahasa Indonesia and English						
Classification within the curriculum:	Compulsory Subject						
Teaching format / class hours per week during the semester:	100 minutes lectures, 120 structured activities and 120 individual study per week						
Workload:	Total workload is 90,67 hours per semester which consists of 100 minutes lectures, 120 structured activities and 120 individual study per week for 16 weeks						
Credit points:	2 SKS (3 ECTS)						
Prerequisites course(s):	Mathematics for Chemistry						
Course Outcomes	After taking this course, the students are expected to be able to: <table border="1" style="margin-left: 20px;"> <tr> <td>CO1</td> <td>Applying the concept of quantum theory in solving problems of chemical research questions</td> </tr> <tr> <td>CO2</td> <td>Explain the results of the analysis of the concept of quantum theory</td> </tr> <tr> <td>CO3</td> <td>Apply the concept of mathematical calculations to answer the problem of quantum chemistry calculations</td> </tr> </table>	CO1	Applying the concept of quantum theory in solving problems of chemical research questions	CO2	Explain the results of the analysis of the concept of quantum theory	CO3	Apply the concept of mathematical calculations to answer the problem of quantum chemistry calculations
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CO2	Explain the results of the analysis of the concept of quantum theory						
CO3	Apply the concept of mathematical calculations to answer the problem of quantum chemistry calculations						
Content:	Quantum Chemistry courses include learning about basic concepts in quantum mechanics, hydrogen atoms, approximation methods, quantum chemical calculations, molecular orbitals and molecular structures and chemical reactions. The subject covers <ol style="list-style-type: none"> 1. Quantum theory and The Wave equation, Atom 2. 3. Basic Methods of Approximation 4. Methods for many-atom systems and their applications 5. Molecular orbital and molecular structure, 6. Orbital theory of reactivity and chemical reactions 						
Study / exam achievements:	Attitude assessment is carried out at each meeting by						

	<p>observation and/or self-assessment techniques using the assumption that basically every student has a good attitude. The student is marked very good or not good attitude if they show it significantly compared to other students in general. The result of attitude assessment is not taken into account in the final grades, but as one of the requirements to pass the course. Students will pass from this course if at least have a good attitude. The final mark will be weight as follow:</p> <table border="1"> <thead> <tr> <th>No</th> <th>CO</th> <th>Assessment Object</th> <th>Assessment Technique</th> <th>Weight</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>CO1, CO2, CO3.</td> <td>a. Participation b. Assignment c. Mid-term exam d. Final Exam</td> <td>Presentation / written test</td> <td>5% 25% 30% 40%</td> </tr> <tr> <td colspan="4">Total</td> <td>100%</td> </tr> </tbody> </table>	No	CO	Assessment Object	Assessment Technique	Weight	1	CO1, CO2, CO3.	a. Participation b. Assignment c. Mid-term exam d. Final Exam	Presentation / written test	5% 25% 30% 40%	Total				100%
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1	CO1, CO2, CO3.	a. Participation b. Assignment c. Mid-term exam d. Final Exam	Presentation / written test	5% 25% 30% 40%												
Total				100%												
Forms of media:	Handout, Board, LCD Projector, Laptop/Computer, Module															
References:	<p>Introductory quantum chemistry (1994): A.K Chandra Quantum Chemistry (2004): Koichi OHNO Ideas of Quantum Chemistry (2007): LUCJAN PIELA Quantum Chemistry (2008): Donald A McQuarrie Quantum Chemistry (2014): Ira N. Levine Undergraduate Quantum Chemistry (2017): Jussi Eloranta Fisika Kuantum (2018): Rustam E. Siregar</p> <p>Suggested Reading: Ariel Caticha. (2018). Entropic Dynamics: Quantum Mechanics from Entropy and Information Geometry. Ann. Phys. (Berlin),1700408 Anton B. Zakharov. (2020). Electronic perturbation effects in the presence of electric field for π-conjugated systems: An electron-correlation study. Int J Quantum Chem 2020; e26260 Mohammad Ghashghaee. (2020). Highly improved carbon dioxide sensitivity and selectivity of black phosphorene sensor by vacancy doping: A quantum chemical perspective. Int J Quantum Chem. 2020; e26265 Thomas E. Albrecht-Schmitt. (2020). Theoretical examination of covalency in berkelium(IV) carbonate complexes. Int J Quantum Chem. 2020; e26254. Meeri Lembinen. (2020). Calculation of core-level electron spectra of ionic liquids. Int J Quantum Chem. 2020;e26247.</p>															

PLO and CO mapping

	PLO										
	Attitude	General Skill			Knowledge				Specific Skill		
	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	PLO8	PLO9	PLO10	
CO1					√						
CO2							√				
CO3									√		