



## 教學計劃表 Syllabus

課程名稱(中文) Course Name in Chinese	無機化學特論 (三)			學年/學期 Academic Year/Semester	113/1			
課程名稱(英文) Course Name in English	Special Topics in Inorganic Chemistry(III)							
科目代碼 Course Code	CHEM72100	系級 Department & Year	博士	開課單位 Course-Offering Department	化學系			
修別 Type	選修 Elective	學分數/時間 Credit(s)/Hour(s)	3.0/3.0					
授課教師 Instructor	/劉鎮維							
先修課程 Prerequisite								

## 課程描述 Course Description

The purpose of this lecture is to teach students in learning X-ray crystallography, which provides detailed 3D structure in atomic resolution for any new crystalline material. Due to the lack of X-ray diffractometer in NDHU, which was unfortunately malfunctioned after the big earthquake on April 3, 2024, I intend to focus on the techniques of solving the structures. The lectures will start at the general introduction of point group symmetry followed by the crystallographic symmetry, which will constitute the lecture materials of the first three weeks. A total of twelve weeks followed are needed to familiarize the SHELXL software in order to solve new structures. This part will be taught by Vincent Liao, a staff crystallographer in the Institute of Chemistry, Academia Sinica. He is willing to share his knowledge and experiences to the Ph. D. students, who are interested in the chemical synthesis.

The students who attend the class must prepare at least one single crystal, which structure has never been deposited in the Cambridge Structure Data Base (CSDB). Obviously the students must own the knowledge searching the CSDB routinely. In addition, the students need to demonstrate in the final examination that they are capable of solving the structure by using the raw data provided by Dr. Vincent Liao. An accompanied Checkcif report without level-A alerts is required to pass the class. After the training, the students will become an expert in evaluating the structure accuracy. Thus if you are not doing the chemical synthesis and will never grow single crystals in your daily bench work, you are not encouraged to attend the class.

## 課程目標 Course Objectives

依照當今無機化學領域之重要發展與本所教師之專長，選擇無機化學領域之中重要主題，進行深入淺出的介紹與研討。

系專業能力 Basic Learning Outcomes		課程目標與系專業能力相關性 Correlation between Course Objectives and Dept.'s Education Objectives
A	具備化學專業知識	●
B	具備設計與執行化學實驗之能力	○
C	具備獨立研究之能	○
D	具備國際競爭力	○

圖示說明 Illustration : ● 高度相關 Highly correlated ○ 中度相關 Moderately correlated

**授課進度表 Teaching Schedule & Content**

週次 Week	內容 Subject/Topics	備註 Remarks
1	The importance of X-ray crystallography in 3D structure determination: case studies	
2	Point group symmetry (Ch. 3) (Cotton's book)	
3	Crystallographic symmetry: 11.1 ~ 11.3 (Cotton's book)	
4	Conquest software Utilizing Conquest software for literature searches within the Cambridge Structural Database (CSD).	
5	Diffraction and crystal structure Introduction to diffraction theory and its application in determining crystal structures.	
6	Crystal system, Bravais lattice, and space groups Exploration of the 7 crystal systems, 14 Bravais lattices and 230 space groups, including their properties and significance.	
7	Miller indices and zone axis symbols Detailed discussion on Miller indices and zone axis symbols, essential for understanding crystal orientation and symmetry.	
8	Crystal growing and screening Techniques for growing and screening crystals suitable for X-ray diffraction analysis.	
9	期中考試週 Midterm Exam	
10	APEX software Hands-on training with APEX software, covering the determination of unit cells, phase-indexing, data collection, absorption correction, and structure solving.	
11	ShelXle software In-depth look at ShelXle software, including its operating principles and key commands for refining crystal structures.	
12	Practical exercises for solving crystal structure Practical sessions focused on solving crystal structures using the skills and software introduced in previous weeks.	
13	Checkcif report, common problems and solution Guidance on generating and interpreting Checkcif reports, with a focus on troubleshooting common issues.	
14	Plotting: Mercury and Diamond Techniques for visualizing and plotting crystal structures using Mercury and Diamond software.	
15	Plotting: Mercury and Diamond Techniques for visualizing and plotting crystal structures using Mercury and Diamond software.	
16	Neutron crystallography Introduction to neutron crystallography, its principles, and applications in determining crystal structures.	
17	The final exam will test students' ability to solve one crystal structure from raw data followed by generating a Checkcif report.	
18	期末考試週 Final Exam	

## 教 學 策 略 Teaching Strategies

課堂講授 Lecture

分組討論 Group Discussion

參觀實習 Field Trip

其他Miscellaneous:

## 教 學 創 新 自 評 Teaching Self-Evaluation

創新教學 (Innovative Teaching)

問題導向學習 (PBL)

團體合作學習 (TBL)

解決導向學習 (SBL)

翻轉教室 Flipped Classroom

磨課師 Moocs

社會責任 (Social Responsibility)

在地實踐 Community Practice

產學合作 Industry-Academia Cooperation

跨域合作 (Transdisciplinary Projects)

跨界教學 Transdisciplinary Teaching

跨院系教學 Inter-collegiate Teaching

業師合授 Courses Co-taught with Industry Practitioners

其它 other:

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### 學期成績計算及多元評量方式 Grading & Assessments

配分項目 Items	配分比例 Percentage	多元評量方式 Assessments						
		測驗 會考	實作 觀察	口頭 發表	專題 研究	創作 展演	卷宗 評量	證照 檢定
平時成績(含出缺席) General Performance (Attendance Record)	50%							
期中考成績 Midterm Exam	10%							
期末考成績 Final Exam	40%							
作業成績 Homework and/or Assignments								
其他 Miscellaneous (_____)								

#### 評量方式補充說明

#### Grading & Assessments Supplemental instructions

The first three lectures (9:10 ~ 12 am) will take place at room D108 (人社學院) and the rest of classes (Tuesday evening, 6 ~ 9 pm) will be taught on line. Both mid-term and final examination will be held in room D108.

#### 教科書與參考書目 (書名、作者、書局、代理商、說明)

Textbook & Other References (Title, Author, Publisher, Agents, Remarks, etc.)

Chemical Applications of Group Theory (3rd edition) by F. A. Cotton. (Chapters 3 & 11)

#### 課程教材網址(含線上教學資訊,教師個人網址請列位於本校內之網址)

Teaching Aids & Teacher's Website (Including online teaching information.

Personal website can be listed here.)

#### 其他補充說明 (Supplemental instructions)