e-learning

X-ray crystallography course

【SCX】 Introduction to single crystal X-ray structure analysis

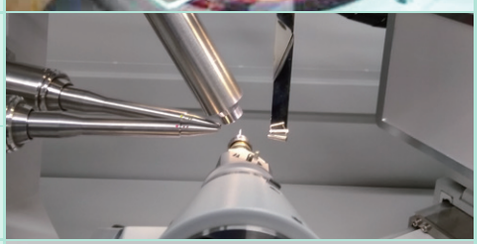
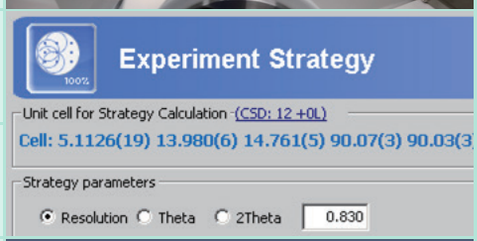
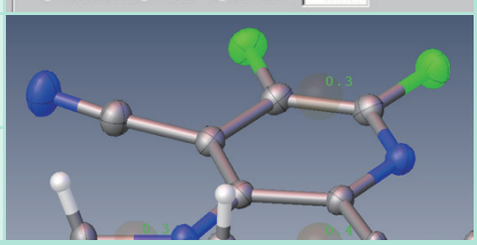
Part number	JHDE004	Required time	Approx. 6 hours*

Single crystal X-ray structure analysis is an indispensable analytical technique that is used not only to determine the three-dimensional structure of novel compounds, but also to understand and utilize their functions.
In this course, you will learn the principles of single crystal X-ray structure analysis and the procedures for growing crystals, measuring X-ray diffraction data and solving a structure, using a small organic compound as a target material. This course is aimed to provide practical knowledge on how to perform X-ray crystallography experiments, so the key technical points of single crystal X-ray structure analysis will be described in detail.

Please note that CrysAlis^{Pro}, our user-inspired data collection and data processing software, and Olex^2, a complete structure solution, refinement and analysis program, are used to describe the use of software in this course.

*The required time is estimated as mininum period by taking consecutive programs from the beginning to the end of the chapters without any repetition.

Learning points

	Introduction Fundamentals of X-ray crystallography	The introduction section briefly describes the basic principles of single crystal X-ray structure analysis and the steps involved.	
Practical Approach (Basic)	Chapter1 Growing crystals	You will learn general procedures to grow high quality crystals of your target sample.	
	Chapter 2 Shaping and mounting crystals	You will learn the techniques of shaping and mounting crystals.	
	Chapter 3 / Chapter 4 Data collection and reduction	You will learn how to collect high quality data and how to examine the results for quality after data reduction.	
	Chapter 5 / Chapter 6 Precedures of structure analysis	You will learn how to proceed with structure solution and refinement to obtain the final structure.	
	Chapter 7 About CIFs - alerts and how to handle them	You will learn how to validate the structure with checkCIF and deal with frequently occurring alerts and their countermeasures.	
Practical Approach (Advanced)	Chapter 1 / Chapter 2 Refinement of disordered structure	You will learn how to define and classify disorder and refine a disordered structure using SHELXL command.	
	Chapter 3 Key points for inverstigation and analysis of twins	You will learn the definitions, types, and warning signs of twinning. Also, you will learn the procedures for data processing, solution and refinement of twinned crystals.	

Appendix

Recent Topics (Technical innovations)	The last section introduces topics related to the latest technical innovations in single crystal X-ray systems.