

---

**Modulbezeichnung:** **Modern X-ray Structure Determination (MXD)** **5 ECTS**  
(Modern X-ray Structure Determination)

Modulverantwortliche/r: Frank Wilhelm Heinemann

Lehrende: Frank Wilhelm Heinemann

---

Startsemester: SS 2022	Dauer: 1 Semester	Turnus: halbjährlich (WS+SS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

---

**Lehrveranstaltungen:**

Modern X-ray structure determination of single crystals (SS 2022, Vorlesung mit Übung, 3 SWS, Frank Wilhelm Heinemann)

---

**Inhalt:**

- Fundamentals of crystallization and polymorphism
- Structural description of single crystals, crystal systems, unit cell, symmetry and symmetry elements, space groups
- Diffraction power of crystals, diffraction conditions, structure factor
- Generation of X-rays, single crystal diffractometers, detection techniques
- Structure solution techniques and refinement procedures, software, problems and pitfalls, interpretation of results
- Anomalous dispersion and absolute structure
- Graphical representations, use of data bases

**Lernziele und Kompetenzen:**

Students ...

- get insight into thermodynamics of crystallization and crystallization techniques
- get fundamentals of the theory behind crystal structure determination
- get practice in crystal selection, mounting and measurement set-up
- get hands-on training in structure solution and refinement using up-to-date software
- are enabled to interpret and compare results of a single crystal structure determination

**Literatur:**

- Werner Massa: Kristallstrukturbestimmung. Teubner Studienbücher Chemie, Vieweg und Teubner, 6. Auflage, 2009, ISBN: 3834806498
- William Clegg: Crystal Structure Determination. Oxford Chemistry Primers. Oxford University Press, 1998, ISBN: 0198559011
- Further literature will be recommended in the course

---

**Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:**

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | NatFak | Chemistry (Master of Science) | Wahlmodule | Modern X-ray Structure Determination)

[2] **Molecular Science (Master of Science): 3. Semester**

(Po-Vers. 2020w | NatFak | Molecular Science (Master of Science) | Elective modules | Modern X-ray Structure Determination)

---

**Studien-/Prüfungsleistungen:**

Modern X-ray Structure Determination (Prüfungsnummer: 65581)

Prüfungsleistung, Übungsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Lab report in manuscript style (max. 2000 words plus raw data); module is ungraded, but has to be passed!

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: keine Angabe

1. Prüfer: Frank Wilhelm Heinemann

---

**Organisatorisches:**

- Module can be taken in winter or in summer term
- Module will be taught in presence and/or online
- Students have to register for the module examination (check registration periods)
- Information/registration available on studon XXXXXXXX

**Bemerkungen:**

Module compatibility:

- as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)