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

Modulverantwortliche/r: Frank Wilhelm Heinemann  
Lehrende: Frank Wilhelm Heinemann

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Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: halbjährlich (WS+SS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

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**Lehrveranstaltungen:**

Modern X-ray structure determination of single crystals (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Frank Wilhelm Heinemann)

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**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

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

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

**[1] Chemistry (Master of Science): ab 3. Semester**

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

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

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

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**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: WS 2021/2022, 1. Wdh.: keine Angabe

1. Prüfer: Frank Wilhelm Heinemann

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**Organisatorisches:**

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

**Bemerkungen:**

Module compatibility:

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