# Moderne Methoden der Strukturbestimmung

Modern Methods of Structure Determination

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# What you will learn..

- Overview of available methods at FU Berlin
- Detailed knowledge on the most important methods

Lectures

- Measurement – Data Analysis – Refinement of Single Crystal Structures
- Measurement – Data Analysis – Evaluation of Powder Patterns

Hands-On Sessions

- Discussion, Presentation and Publication of Structure Results

Exam

# When and what and where?

**Lectures**

Tuesdays, 1pm – 5pm, Seminar Room (check which one on homepage), Everyone

**Hands-On Sessions**

24.10 – 12.11 groups of three, each group one evening (5pm)
online signup (link: homepage AG Thiele)
@basement, meeting in front of the elevator.

13.11, 20.11, 04.12 Instead of the Lecture (Seminar Room, 1pm – 5pm)

**Exam**

18.02 – 22.02 (online signup)
groups of three, 45 minutes per group
Presentation of the Refinement, the Publication, and discussion of the suitable analytics.

# Time Schedule

Oktober

| | M | D | M | D | F | S | S |
|---|---|---|---|---|---|---|---|
| 40 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| 41 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
| 42 | 15 | 16 | 17 | 18 | 19 | 20 | 21 |
| 43 | 22 | 23 | 24 | 25 | 26 | 27 | 28 |
| 44 | 29 | 30 | 31 | 1 | 2 | 3 | 4 |
| 45 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |

November

| | M | D | M | D | F | S | S |
|---|---|---|---|---|---|---|---|
| 44 | 29 | 30 | 31 | 1 | 2 | 3 | 4 |
| 45 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| 46 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
| 47 | 19 | 20 | 21 | 22 | 23 | 24 | 25 |
| 48 | 26 | 27 | 28 | 29 | 30 | 1 | 2 |
| 49 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |

Dezember

| | M | D | M | D | F | S | S |
|---|---|---|---|---|---|---|---|
| 48 | 26 | 27 | 28 | 29 | 30 | 1 | 2 |
| 49 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| 50 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
| 51 | 17 | 18 | 19 | 20 | 21 | 22 | 23 |
| 52 | 24 | 25 | 26 | 27 | 28 | 29 | 30 |
| 1 | 31 | 1 | 2 | 3 | 4 | 5 | 6 |

Januar

| | M | D | M | D | F | S | S |
|---|---|---|---|---|---|---|---|
| 1 | 31 | 1 | 2 | 3 | 4 | 5 | 6 |
| 2 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
| 3 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| 4 | 21 | 22 | 23 | 24 | 25 | 26 | 27 |
| 5 | 28 | 29 | 30 | 31 | 1 | 2 | 3 |
| 6 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |

Februar

| | M | D | M | D | F | S | S |
|---|---|---|---|---|---|---|---|
| 5 | 28 | 29 | 30 | 31 | 1 | 2 | 3 |
| 6 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| 7 | 11 | 12 | 13 | 14 | 15 | 16 | 17 |
| 8 | 18 | 19 | 20 | 21 | 22 | 23 | 24 |
| 9 | 25 | 26 | 27 | 28 | 1 | 2 | 3 |
| 10 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |

März

| | M | D | M | D | F | S | S |
|---|---|---|---|---|---|---|---|
| 9 | 25 | 26 | 27 | 28 | 1 | 2 | 3 |
| 10 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| 11 | 11 | 12 | 13 | 14 | 15 | 16 | 17 |
| 12 | 18 | 19 | 20 | 21 | 22 | 23 | 24 |
| 13 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
| 14 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |

Lecture

Diffraction Time

Exam

# Lectures: Tuesdays, 1pm – 5pm

**Q&A Session for Installations: 06.11. 5pm**

| | | |
|---|---|---|
| 16.10.2018 | Organization and Overview Methods | Thiele |
| 23.10.2018 | Theory of Single Crystal Structure Determination | Thiele |
| 30.10.2018 | Theory of Single Crystal Structure Determination | Thiele |
| 06.11.2018 | Theory of Single Crystal Structure Determination | Thiele |
| 13.11.2018 | Hands-on Session Refinement | Thiele/Steinhauer/Hagenbach |
| 20.11.2018 | Hands-on Session Refinement | Thiele/Steinhauer/Hagenbach |
| 04.12.2018 | Publication Training | Thiele/Steinhauer/Hagenbach |
| 11.12.2018 | Powder Diffraction, Energy Dispersion and X-Ray Fluorescence | Thiele |
| 18.12.2018 | Solid State NMR | Steinhauer |
| 08.01.2019 | Electrochemical Methods | Sarkar |
| 15.01.2019 | Electron Pair Resonance | Sarkar |
| 22.01.2019 | Mass spectrometry | Springer |
| 29.01.2019 | IR/Raman/Matrix/IMMS | Riedel/Pagel |
| 05.02.2019 | UV-Vis/Fluorescence | Kulak |

**Laptops!**

# Single Crystal Structure Determination

1) Synthesis of Compounds
2) Crystallization

3) Sample Preparation
4) Sample Measurement

5) Data Integration
6) Structure Refinement

7) Structure Analysis, Presentation
8) Structure Publication

## Do it Yourself

**@basement**
**First evening 5:45 pm**

**Second evening 5:15 pm**
**Tuesday's Hands-On Sessions**

**Tuesday's Hands-On Sessions**
**Exam**

# How to crystallize?

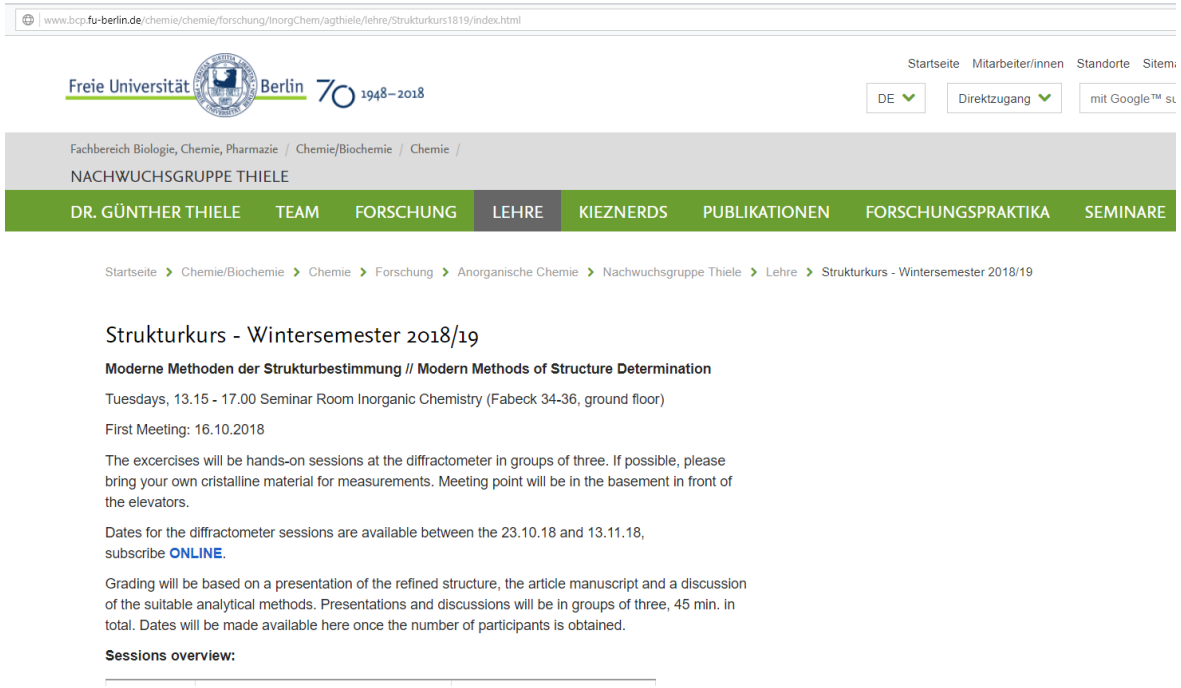
- Solvent evaporation
- Solvent diffusion
- Temperature gradient
- Concentration gradient

**The slower the Crystallization Process, the better the Crystal Quality!**

Ideal Crystal Size for the IPDS 2T: 1 mm each side

# Information & Slides & Online SignUp

Homepage FU Berlin > BCP > Chemie > AG Thiele > Lehre > Strukturkurs




# Your To-Do-List

1) Crystallize something
2) Set up your laptop
3) Find your group (three people)
4) SignUp Online for Diffraction time
5) SignUp @ BlackboardFU
   or on paper (“alte Prüfungsordnung“)

For the diffraction time:
At the sign-up date: be there at 5:45 pm with your crystals
The next day: be there at 5:15 pm with your crystals (PXRD)

# Questions ?

This Modul will be evaluated (January?). Please participate to give your input on how to improve it.