Quantitative Phase Analysis by Rietveld Method

Theory and hands-on short course

Program

Day 1

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 ***Introductory crystallography:*** unit cell, symmetry elements of macro- and microcrystallography, crystal structures, seven crystal systems, 14 Bravais lattices, space groups

10:30 – 11:50 Coffee Break

11:50 – 13:00 ***X-ray diffraction:*** Miller indices, atomic scattering factors, anomalous dispersion; X-ray sources, choice of radiation, wavelength, resolution, mass absorption,

13:00 – 14:00 Lunch

14:00 – 15:30 **Modeling** ***of powder diffraction data.*** Integrated intensities, peak position and peak intensity,

15:30 – 15:50 Coffee Break

15:50 – 17:00 ***Database and phase identification (Practical sessions)***

Day 2

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 ***Least square fitting:*** zero, unit cell, background, halfwidths, peak shape, proffered orientation,

10:30 – 11:50 Coffee Break

11:50 – 13:00 ***Corrections:***

13:00 – 14:00 Lunch

14:00 – 15:30 ***No Structural Data:***

15:30 – 15:50 Coffee Break

15:50 – 17:00 ***New structural data:***

Day 3

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 ***SIROQUANT- strategy, capabilities, demonstration***

10:30 – 11:50 Coffee Break

11:50 – 13:00 ***SIROQUANT (exercises)***

13:00 – 14:00 Lunch

14:00 – 15:30 **TOPAS** ***strategy, capabilities, demonstration***

15:30 – 15:50 Coffee Break

15:50 – 17:00 ***TOPAS (exercises)***

Day 4

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 ***RIQAS strategy, capabilities, demonstration***

10:30 – 11:50 Coffee Break

11:50 – 13:00 ***RIQAS (exercises)***

13:00 – 14:00 Lunch

14:00 – 15:30

15:30 – 15:50 Coffee Break

15:50 – 17:00

Standardless quantitative phase analysis of X-ray powder diffraction data by the Rietveld method-why benefits:

Rietveld analysis of X-ray powder diffraction data can be utilized for the determination of the quantitative phase composition of inorganic crystalline raw materials, materials of natural origin (soils, rocks), intermediate products, precursor phases or of final products

It helps:

- To manufacture ***products with reproducible quality*** for producing and processing industries.
- To ensure a constant quality the ***specific properties of the material*** have to be defined and controlled.
- Often the ***mineralogical phase composition*** is one of the most decisive and measurable factors of quality.
- To control by the supplier of the raw materials during the process
- To control of the producer of half wares or final products during (**process control**) and after the production (**quality control of the product**).
- Control by the customer of raw materials, half wares or final products (**income control of the material**).

For academic research, government and industry

Cement clinker and cement
Limestone and lime based products
Gypsum- and anhydrite based products
Mixtures of different building materials
Intermediate and final ceramic materials
Refractory materials
Natural and synthetic inorganic raw materials
Pharmaceutical Industry
Active pharmaceutical ingredient or testing of the pharmaceutical product
Polymorphic purity, state of hydration, degree of crystallinity and/or particle size of the active pharmaceutical product
Analysis of the composition of a tablet or tablet components