# Powder pattern matching with Crystallography Open Database

# Powder pattern matching with Crystallography Open Database

- COD (http://www.crystallography.net/cod/) has a large set of crystal structures

- Powder patterns have been simulated for all crystal structures and collected into a database that can be used for pattern matching and phase identification

- Has been integrated in some commercial programs (Rigaku, PANalytical, Match!) and with free QualX2 program (http://www.ba.ic.cnr.it/softwareic/qualx/)

- Full Profile Search Match web service is available at http://nanoair.dii.unitn.it:8080/sfpm/

*Full Profile Search Match*

by L. Lutterotti using COD

# Example with ZnO (1)

- Let's try the Full Profile Search Match web service with ZnO as an example
  - Download Powder XRD data ZnO-test.xy located in
    MyCourses -> Databases -> Full Profile Search Match (Powder COD)

### Diffraction pattern and sample characteristics

Upload diffraction pattern: [ Choose File ] 2107059.xy

Structures db: [ COD_all.sqlite ▼ ] ☑ mineral ☑ inorganic ☐ organic ☐ metalorganic ☐ other

Atomic elements in the sample:
[ Zn O ]

Threshold phase density [ 2 ]   Threshold remove: [ 0.01 ]   Phases maximum number: [ 4 ]

Crystallisation: [ normal ▼ ]   ☑ Cell parameters isotropic expansion/contraction

**1. Select both *mineral* and *inorganic***

**2. Limit elements**

**3. Increase density threshold to 2 g/cm³**

**4. Limit the number of phases to 4 or less**

### Experiment details

Radiation:
⦿ X-ray tube: [ Cu ▼ ]
◯ Other : [ x-ray ▼ ] Wavelength (Å): [ 1.540598 ]

Instrument geometry:
⦿ Bragg-Brentano (theta-2theta)
◯ Bragg-Brentano (2theta only), omega: [ 10 ]
◯ Debye-Scherrer
◯ Transmission

Instrument broadening function: [ Medium ▼ ]

**5. Try *medium* broadening first. If this does not give reasonable matches, try *high* broadening**

### Algorithm options (Rietveld, ddm or both)

Weights type: [ -1 ]   Smooth weight: [ 0 ]   1st weight: [ 1 ]   2nd weight: [ 1 ]

[ Search and quantify ]

3

# Example with ZnO (2)

- The search will match with ZnO. You may sometimes get unreasonable matches with small contributions (few weigth %). You can typically disregard those.
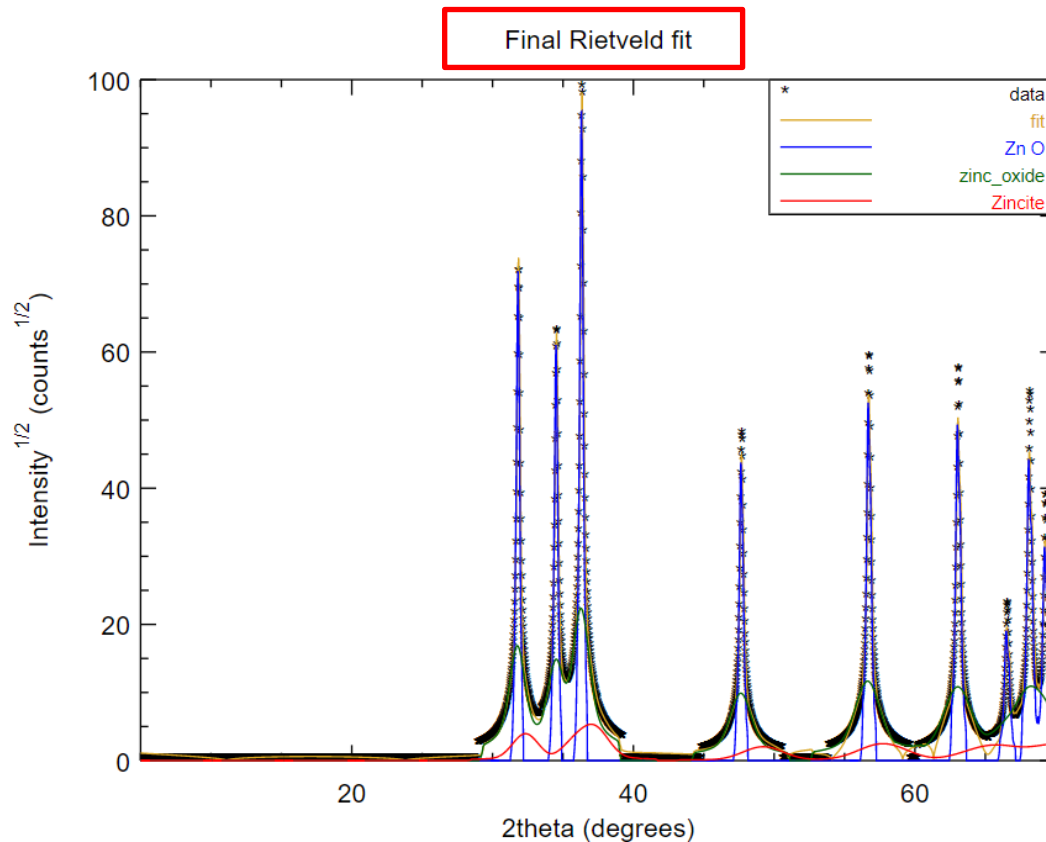
Found phases and quantification:

**Click to get the database entry in COD**

| Phase COD ID | cif file | name | vol. (%) | wt. (%) | crystallites (Å) | microstrain |
|---|---|---|---|---|---|---|
| 2107059 | 2107059.cif | Zn O | 76.5139 | 76.0044 | 1732.63 | 0.000535982 |
| 2300115 | 2300115.cif | zinc_oxide | 21.792 | 22.4323 | 189.295 | 0.008173 |
| 1011259 | 1011259.cif | Zincite | 1.69413 | 1.56329 | 825.776 | 0.018767 |

Final Rietveld analysis, Rw: 0.235555, GofF: 1.67017

**Information card for entry 2107059**

2107058 << **2107059** >> 2107060

**Preview**



Final Rietveld fit

HM:P 63 m c #186
a=3.242Å
b=3.242Å
c=5.188Å
α=90.000°
β=90.000°
γ=120.000°

JSmol
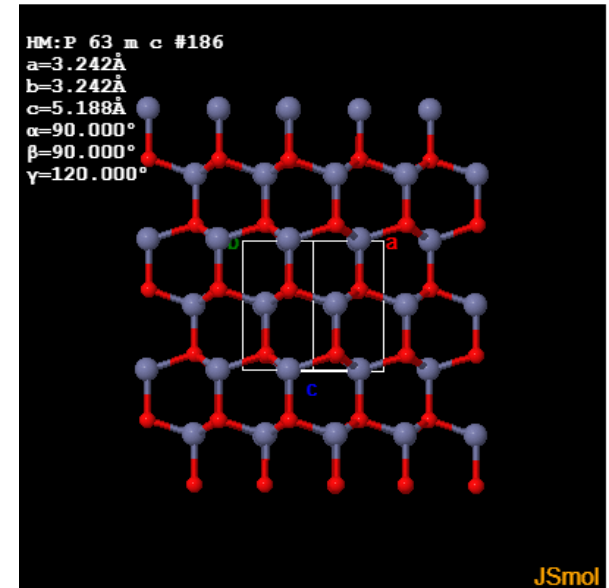
**Coordinates**    2107059.cif

4