

AK Eychmüller GroupSeminar

Brief introduction to the
WinXPow for XRD.

AK Eychmüller GroupSeminar

Brief introduction to the WinXPow for XRD.

Professuren der Fachrichtung Chemie und Lebensmittelchemie - Mozilla Firefox

Datei Bearbeiten Ansicht Chronik Lesezeichen Extras Hilfe

http://www.chm.tu-dresden.de/pc2/eintern.shtml

TECHNISCHE UNIVERSITÄT DRESDEN Physical Chemistry/Electrochemistry

TU Dresden » Faculty of Science » Department of Chemistry and Food Chemistry » PC2

GROUP


- Start
- News
- Events
- Members
- WG Bund
- Jobs Vacancies
- Internal Info

RESEARCH

- Nanocrystals
- Projects
- Publications
- Cooperations

TEACHING

- Overview
- Lectures
- Exercises
- Practical Training
- Miscellanea



@akeychm excursion 2007

important links

Information system on hazardous substances

- [Databases on hazardous substances of BGIA](#)
- [material safety data sheet of euSDB](#)

important contact

- [Glassblower](#)

Analysis and Service (Department of chemistry)

- [Overview of measurements and equipment](#)
- [Measuring data service](#)
- [nanoeva](#)

downloads

Seminar - on wednesdays at 9.30 a.m./room 302/E.-Müller-Bau

- [current seminar plan](#)


Ordering and application form

- [Order form of XRD-measurements](#)
- [Chemicals ordering](#)
- [POSTERPRINT-instruction](#)

Safety and Disposal

- [Eye and lab shower controle](#)
- [Solvent Disposal and Refill](#)

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Wissen schafft Brücken.

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Brief introduction to the WinXPow for XRD.

Serviceauftrag Röntgenografische Messung an Pulvern (XRD)	
Name des Auftraggebers:	Datum:
Arbeitsgruppe: AK Eychmüller	Telefon:
Instrument: Physikalische Chemie/ Elektrochemie	
Kostenstelle:	
Email:	
Probenbezeichnung:	
Messtemperatur:	
Probenanordnung: <input type="checkbox"/> Transmission <input type="checkbox"/> Reflexion <input type="checkbox"/> Kapillare	
Diffraktometer: <input type="checkbox"/> Siemens D5000 <input type="checkbox"/> STOE STADI-P (IP) <input type="checkbox"/> STOE STADI (PSD) <input type="checkbox"/> SAXS Nanostar (Small-Angle-X-ray-Scattering)	
Spezielle Blenden/ Kollimatoren/ Probenträger:	
Messbereich 2 θ min./ 2 θ max.:	
Messdauer: Übersichtsmessung Nachtmessung (ca. 12h)	
Ausgabeformat: Messfile (raw)/ ASCII-File/ Grafik (WMF)/ plt.- Format (nur bei SAXS Nanostar)	*.raw
Bemerkungen:	Unterschrift Auftraggeber:
Kosten:	Bearbeiter:

Spezielle Blenden/ Kollimatoren/ Probenträger:	
Messbereich 20 min./ 20 max.:	
Messdauer: Übersichtsmessung Nachtmessung (ca. 12h)	
Ausgabeformat: Messfile (raw)/ ASCII-File/ Grafik (WMF)/ plt.- Format (nur bei SAXS Nanostar)	*.raw
Bemerkungen:	Unterschrift Auftraggeber:
Kosten:	Bearbeiter:

Mailprograms destroy .raw-files!! (Thunderbird, Outlook, etc.)

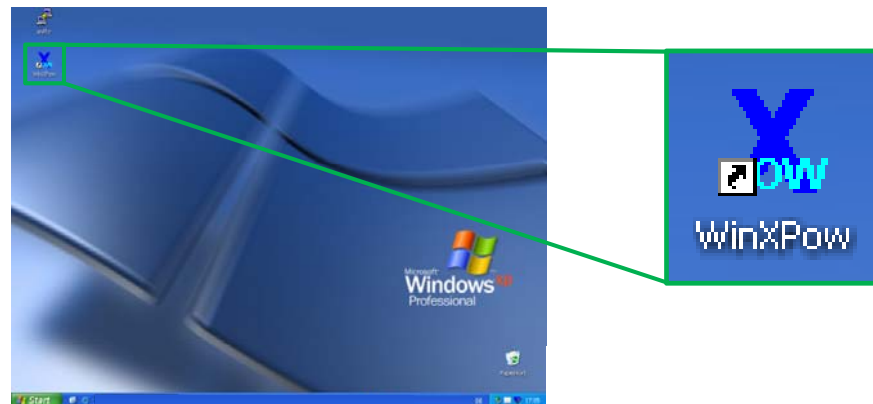
⇒ downloading from:

1. Measuring Data Service
2. Squirrel Mail

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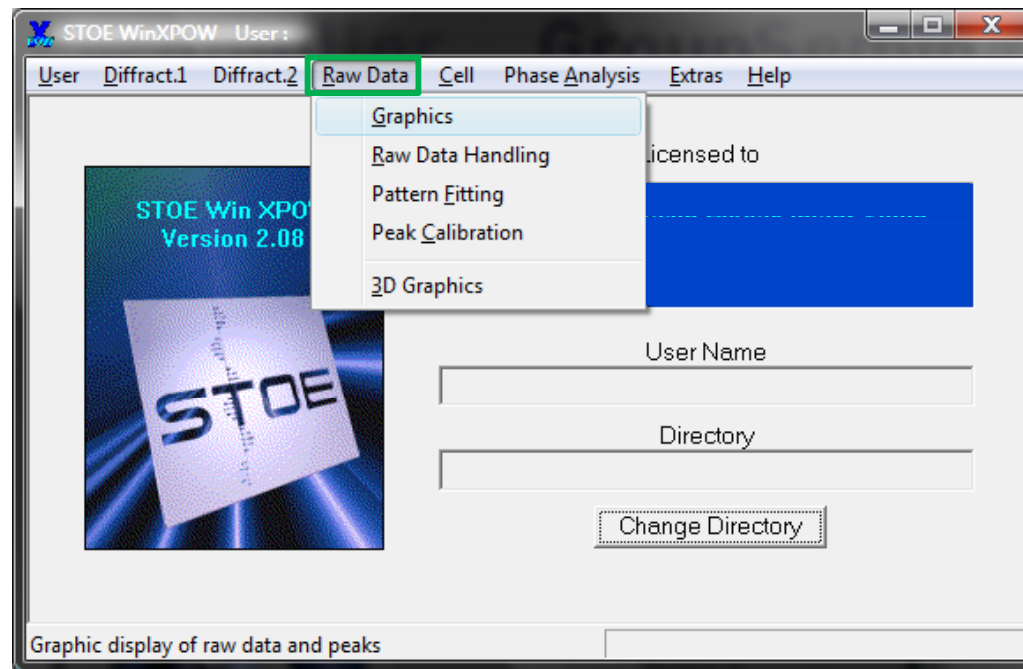
Brief introduction to the WinXPow for XRD.

- Licenced to:
Professorship of the Inorganic Chemistry
Prof. S. Kaskel
- Permission for us:
installation on one computer for the hole group
⇒ office R 003
⇒ user: office03
⇒ psw: useropen



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Brief introduction to the WinXPow for XRD.



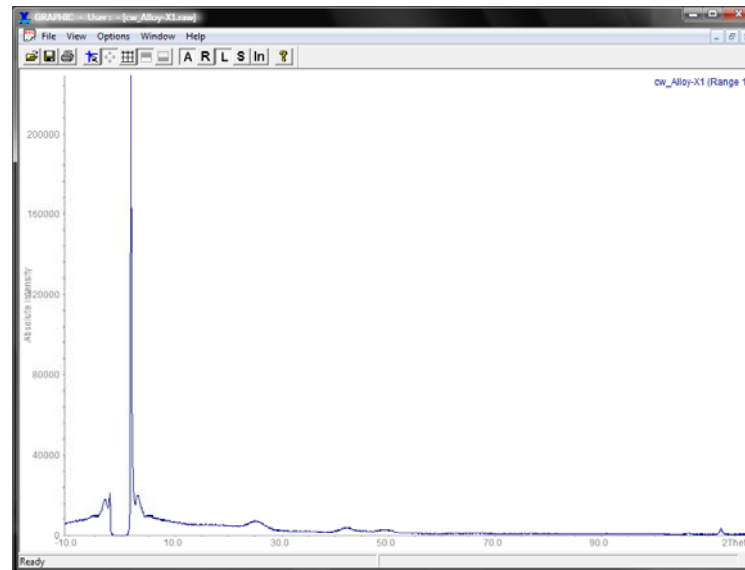
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Brief introduction to the WinXPow for XRD.

- Raw Data → Graphics

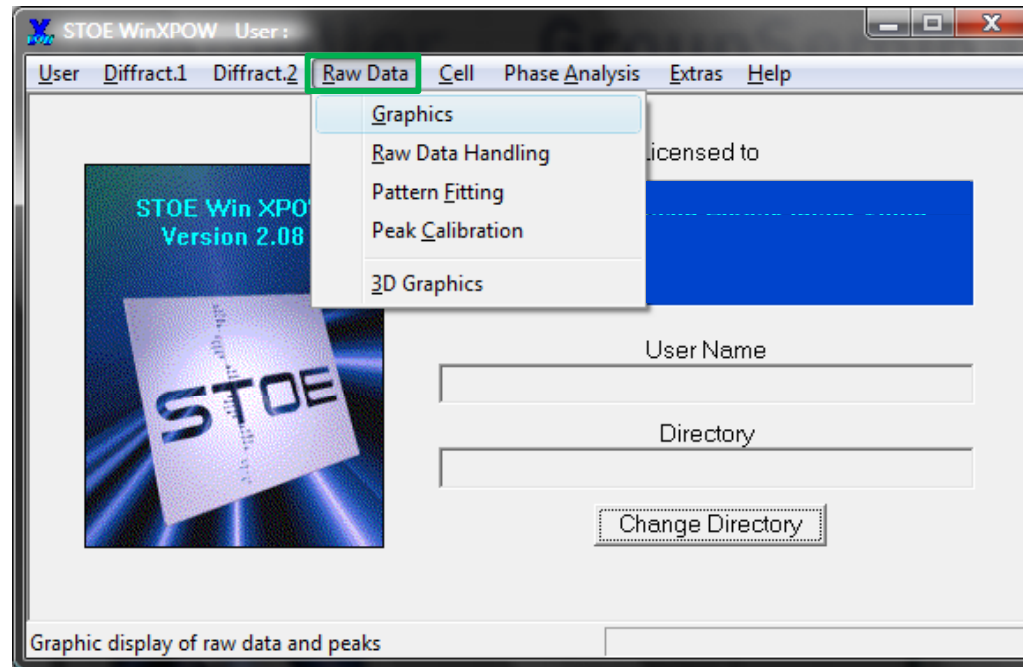


- File → Open → cw_Alloy-X1.raw



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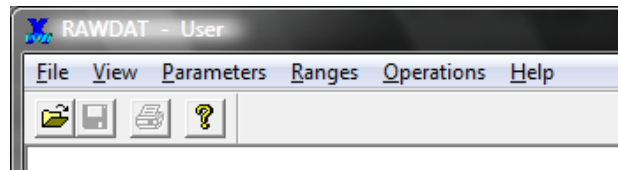
Brief introduction to the WinXPow for XRD.



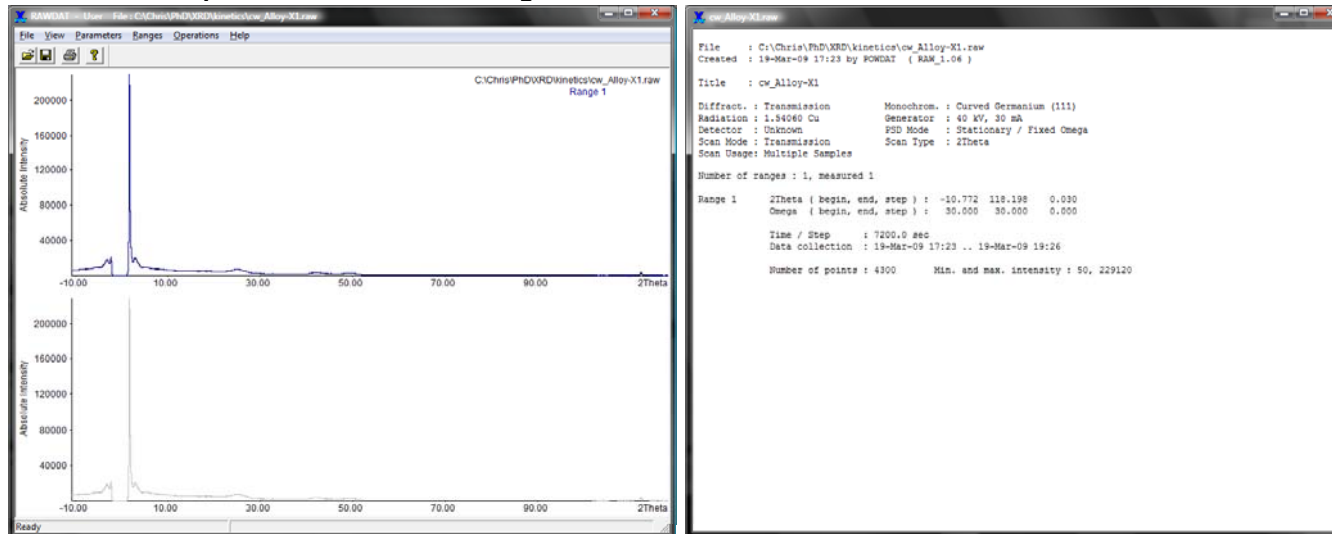
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Brief introduction to the WinXPow for XRD.

- Raw Data → Raw Data Handling



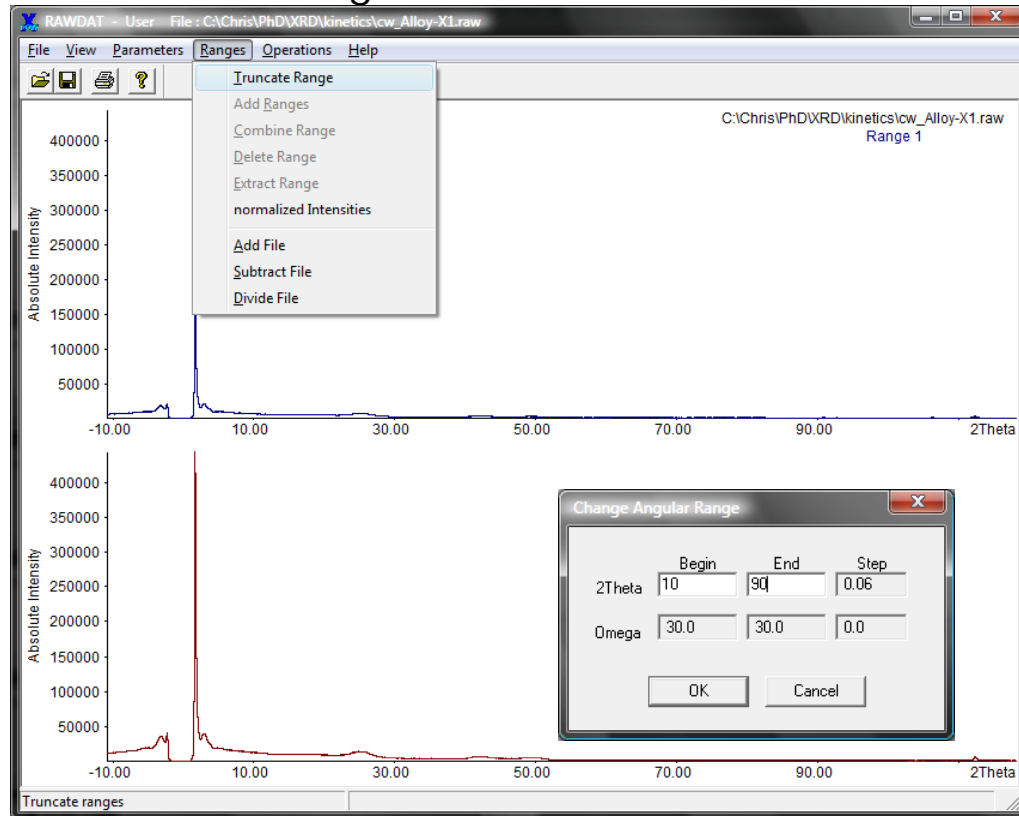
- File → Open → cw_Alloy-X1.raw



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Brief introduction to the WinXPow for XRD.

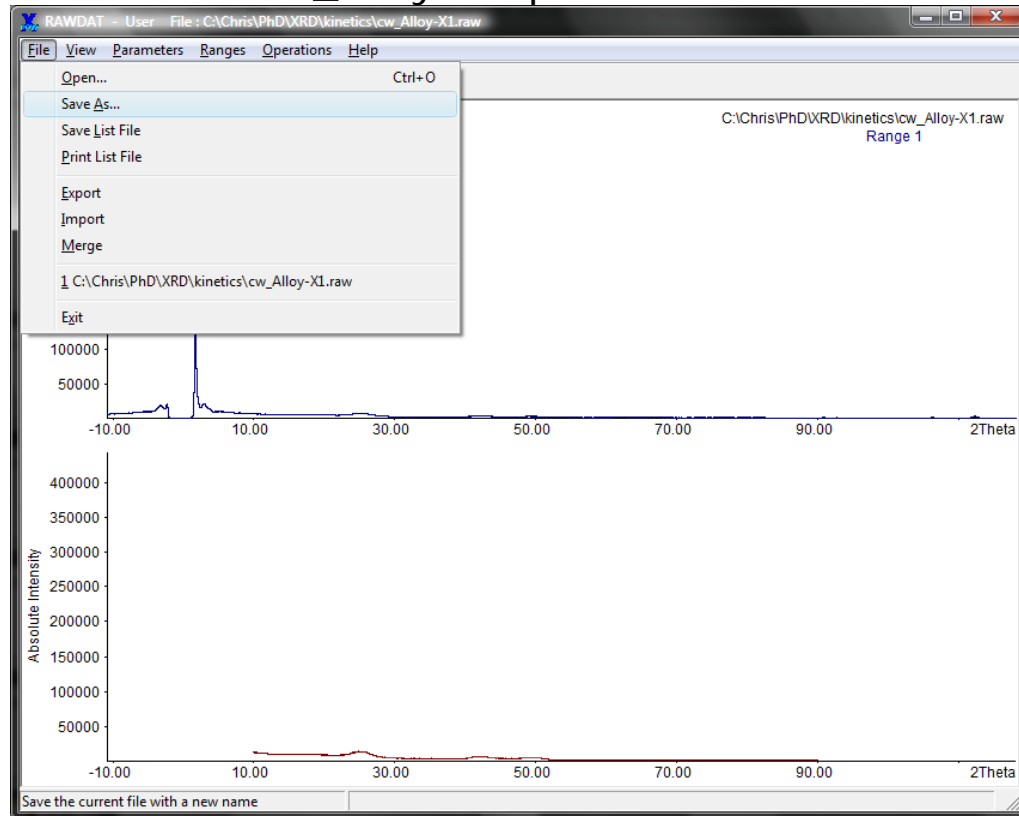
- Ranges → Truncate Range → 2Theta: 10 to 90



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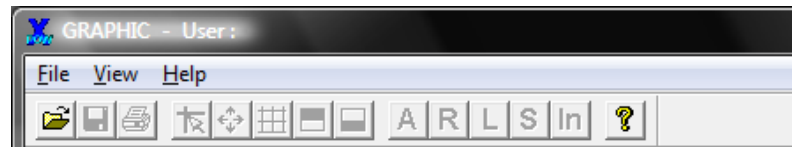
- File → Save As → cw_Alloy-X1opt.raw



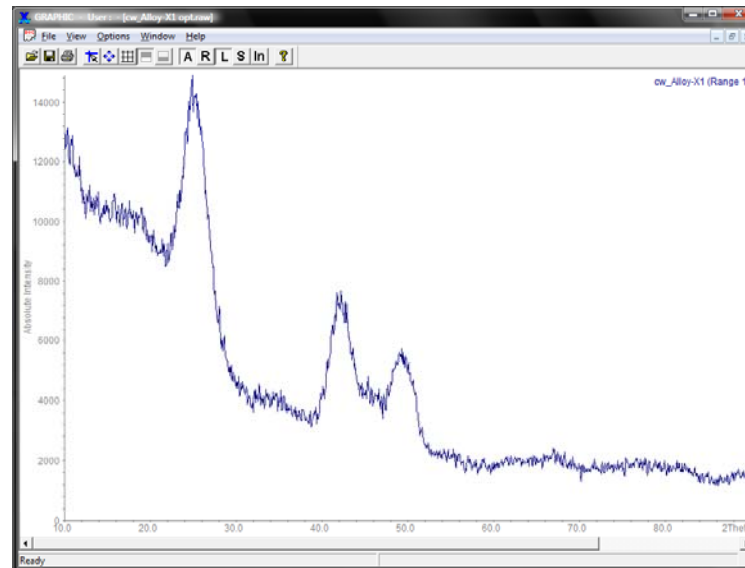
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Brief introduction to the WinXPow for XRD.

- Raw Data → Graphics

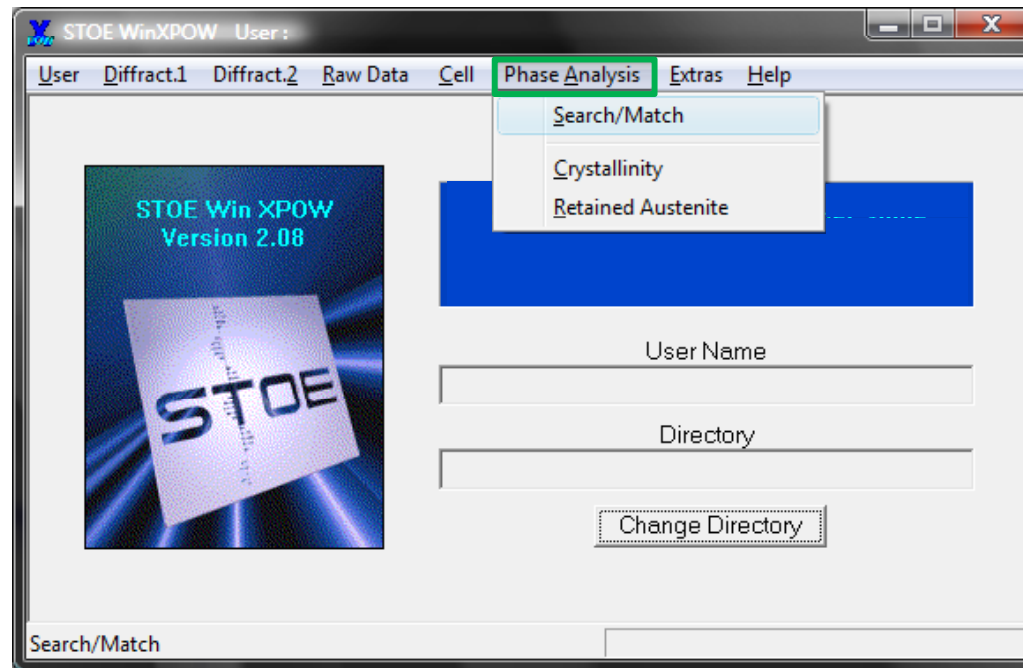


- File → Open → cw_Alloy-X1opt.raw



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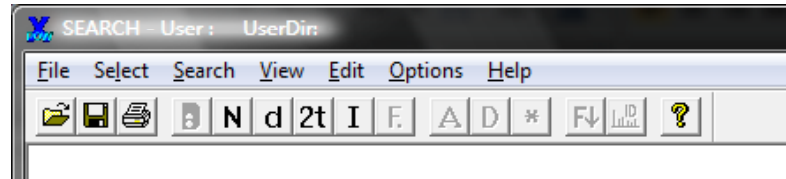
Brief introduction to the WinXPow for XRD.



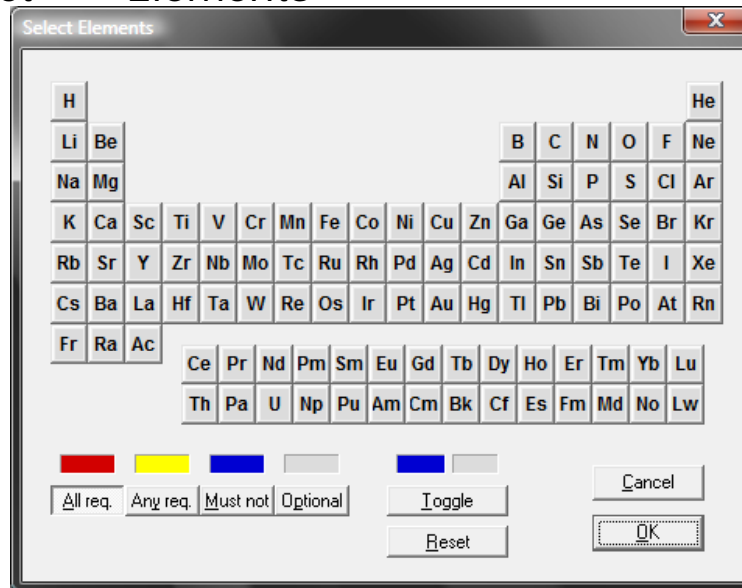
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Brief introduction to the WinXPow for XRD.

- Phase Analysis → Search Match



- Select → Elements

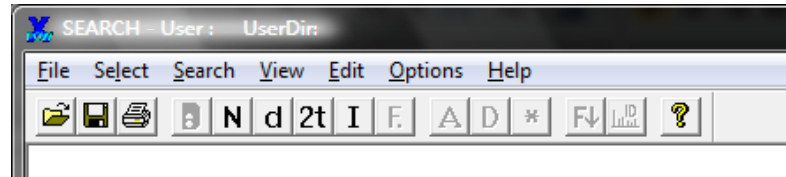


1. press **Toggle**

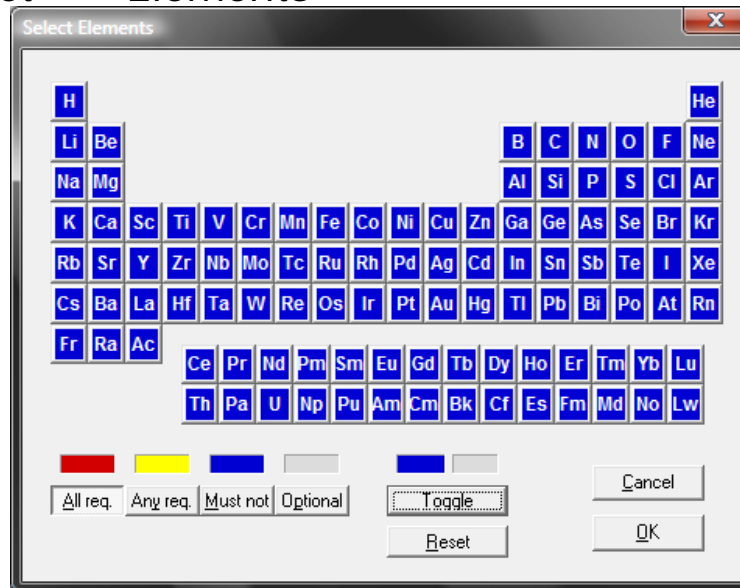
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Brief introduction to the WinXPow for XRD.

- Phase Analysis → Search Match



- Select → Elements

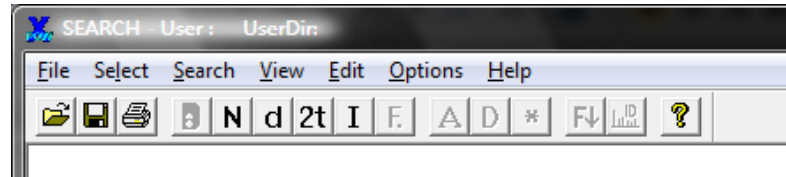


1. press **Toggle**
2. select **All required elements**

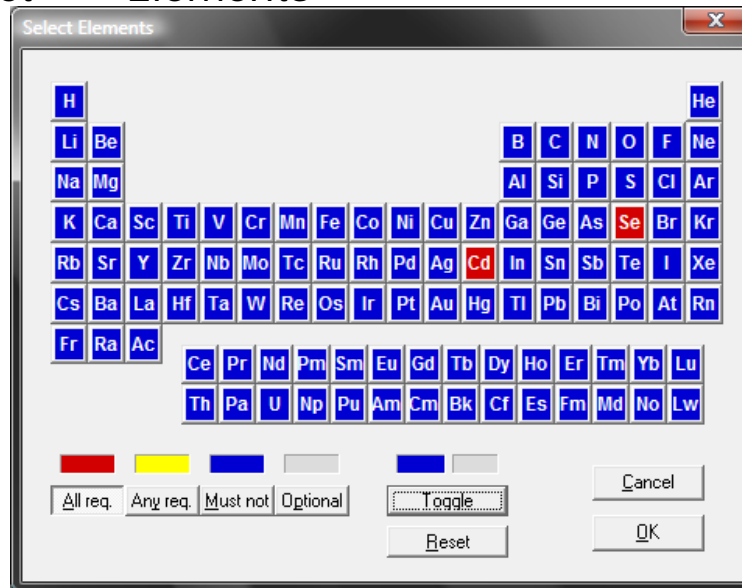
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Brief introduction to the WinXPow for XRD.

- Phase Analysis → Search Match



- Select → Elements

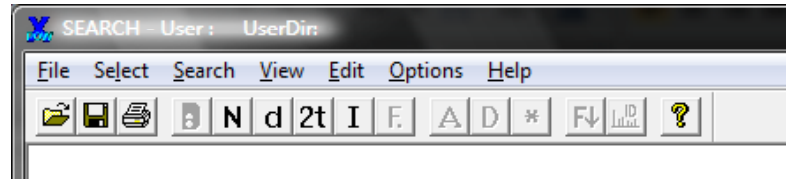


1. press **Toggle**
2. select **All required elements**
3. press **OK**

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Brief introduction to the WinXPow for XRD.

- Phase Analysis → Search Match



- Select → Elements

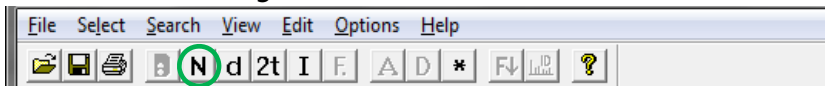


1. press **Toggle**
2. select **All required elements**
3. press **OK**
4. press **Replace**

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Brief introduction to the WinXPow for XRD.

- Phase Analysis → Search Match



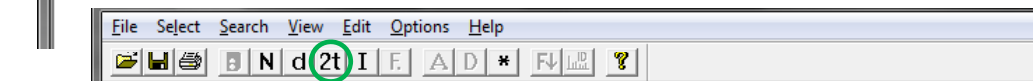
view Names

```
1 [ 8- 459] Cd Se / Cadmium Selenide / Cadmoselite, syn
2 [19- 191] Cd Se / Cadmium Selenide
```



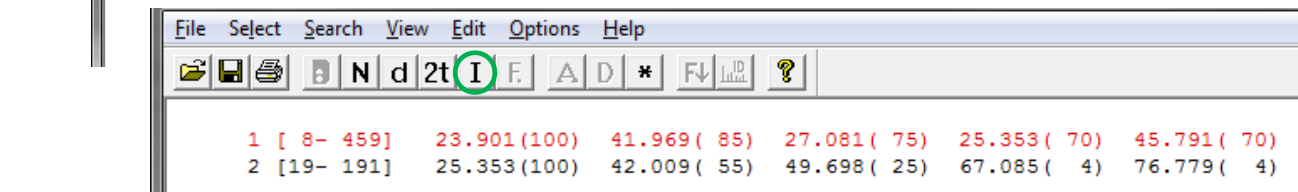
view d-values

```
1 [ 8- 459] 3.720(100) 3.510( 70) 3.290( 75) 2.554( 35) 2.151( 85)
2 [19- 191] 3.510(100) 2.149( 55) 1.833( 25) 1.519(  2) 1.394(  4)
```



view 2theta °

```
1 [ 8- 459] 23.901(100) 25.353( 70) 27.081( 75) 35.108( 35) 41.969( 85)
2 [19- 191] 25.353(100) 42.009( 55) 49.698( 25) 60.942(  2) 67.085(  4)
```



view intensities

```
1 [ 8- 459] 23.901(100) 41.969( 85) 27.081( 75) 25.353( 70) 45.791( 70)
2 [19- 191] 25.353(100) 42.009( 55) 49.698( 25) 67.085(  4) 76.779(  4)
```

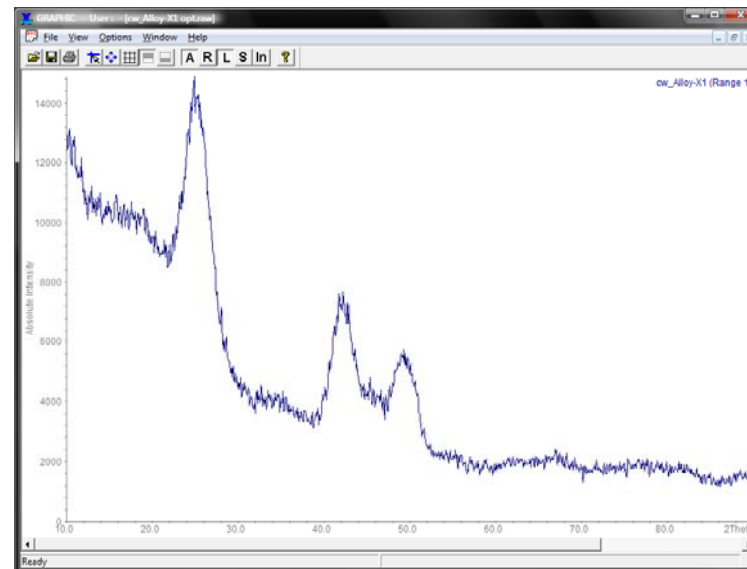
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Brief introduction to the WinXPow for XRD.

- Raw Data → Graphics



- File → Open → cw_Alloy-X1opt.raw



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Brief introduction to the WinXPow for XRD.

- Right Mouse Button:

Add Raw Data	to overlay different *.raw-files
Add Peak Data	to overlay a theoretical pattern or *.pks-file
Add ICDD Data	to overlay a theoretical pattern from the ICDD Data
Split	split the screen
Scaling Axes	scales the axis
Edit Curves ...	option to delete overlayed data
Insert Note ...	insert a note

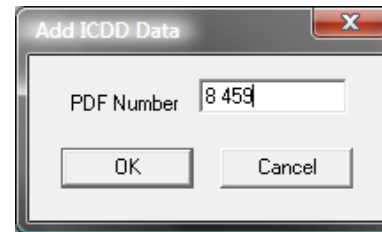
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Brief introduction to the WinXPow for XRD.

- Right Mouse Button → Add ICDD Data

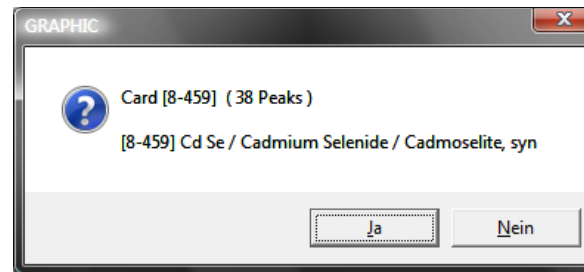
type in the number with space or komma

→ OK



Right number? Correct substance?

→ Ja



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Brief introduction to the WinXPow for XRD.

- Right Mouse Button → Add ICDD Data

Right number! Correct substance!



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Brief introduction to the WinXPow for XRD.

- Right Mouse Button → Add ICDD Data

Right number! Correct substance!



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Brief introduction to the WinXPow for XRD.

- Shut down WinXPow:

first:

close every working window (e.g. GRAPHICS, SEARCH/MATCH)

last:

close MAIN MENU

