This is the simple example template containing only headers for each report item and the bookmarks. The invisible bookmarks are indicated by text between brackets.

Modify it according to your own needs and standards.

## Measurement Conditions: (Bookmark 1)

Dataset Name sample #1

File name C:\Users\Chris Pratt\Desktop\Summer 2017\sample #1.xrdml

Measurement Start Date/Time 9/30/2013 9:38:59 AM

Operator Philips MPD

Raw Data Origin XRD measurement (\*.XRDML)

Scan Axis Gonio

Start Position [°2θ] 10.0100

End Position [°2θ] 129.9900

Step Size [°2θ] 0.0200

Scan Step Time [s] 5.0000

Scan Type Continuous

Offset [°2θ] 0.0000

Divergence Slit Type Fixed

Divergence Slit Size [°] 0.8059

Specimen Length [mm] 10.00

Receiving Slit Size [mm] 0.4500

Measurement Temperature [°C] 25.00

Anode Material Cu

K-Alpha1 [Å] 1.54060

K-Alpha2 [Å] 1.54443

K-Beta [Å] 1.39225

K-A2 / K-A1 Ratio 0.50000

Generator Settings 30 mA, 40 kV

Diffractometer Type 0000000000000000

Diffractometer Number 0

Goniometer Radius [mm] 173.00

Dist. Focus-Diverg. Slit [mm] 91.00

Incident Beam Monochromator No

Spinning No

## Main Graphics, Analyze View: (Bookmark 2)



## Peak List: (Bookmark 3)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Pos. [°2θ] | Height [cts] | FWHM Left [°2θ] | d-spacing [Å] | Rel. Int. [%] |
| 28.5179 | 72248.55 | 0.1378 | 3.13001 | 100.00 |
| 47.3783 | 40531.58 | 0.0960 | 1.91724 | 56.10 |
| 56.1835 | 19011.58 | 0.1200 | 1.63585 | 26.31 |
| 69.1850 | 5356.42 | 0.1200 | 1.35679 | 7.41 |
| 76.4496 | 9078.34 | 0.1200 | 1.24493 | 12.57 |
| 88.0846 | 8659.68 | 0.1440 | 1.10804 | 11.99 |
| 95.0133 | 4364.21 | 0.1440 | 1.04468 | 6.04 |
| 106.7627 | 3602.28 | 0.1440 | 0.95973 | 4.99 |
| 114.1449 | 5108.63 | 0.1680 | 0.91772 | 7.07 |
| 127.5840 | 3596.87 | 0.2160 | 0.85856 | 4.98 |

## Pattern List: (Bookmark 4)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Visible | Ref. Code | Score | Compound Name | Displacement [°2Th.] | Scale Factor | Chemical Formula |
| \* | 00-027-1402 | 100 | Silicon | 0.059 | 0.942 | Si |

## Document History: (Bookmark 5)

Insert Measurement:

- File name = "sample #1.xrdml"

- Modification time = "7/7/2017 2:24:43 PM"

- Modification editor = "Chris Pratt"

Default properties:

- Sample name = ""

- Sample prepared by = ""

- Measurement step axis = "None"

- Sample mode = "Reflection"

- Internal wavelengths used from anode material: Copper (Cu)

- Original K-Alpha1 wavelength = "1.54056"

- Used K-Alpha1 wavelength = "1.54060"

- Original K-Alpha2 wavelength = "1.54439"

- Used K-Alpha2 wavelength = "1.54443"

- Original K-Beta wavelength = "1.39222"

- Used K-Beta wavelength = "1.39225"

- Dist. focus to div. slit = "91.00000"

- Irradiated length = "10.00000"

- Spinner used = "No"

- KBeta filter material = "Ni"

- KBeta filter thickness = "0.02000"

- Linear detector mode = "None"

- Length linear detector = "2"

- Step axis value = "0.00000"

- Offset = "0.00000"

- Sample length = "10.00000"

- Modification time = "7/7/2017 2:24:43 PM"

- Modification editor = "Chris Pratt"

Determine Background:

- Add to net scan = "Nothing"

- User defined intensity = "-5"

- Correction method = "Automatic"

- Bending factor = "0"

- Minimum significance = "0.7"

- Minimum tip width = "0"

- Maximum tip width = "1"

- Peak base width = "2"

- Use smoothed input data = "Yes"

- Granularity = "16"

- Modification time = "7/7/2017 2:27:15 PM"

- Modification editor = "Chris Pratt"

Search Peaks:

- Minimum significance = "2"

- Minimum tip width = "0.00999999977648258"

- Maximum tip width = "1"

- Peak base width = "2"

- Method = "Minimum 2nd derivative"

- Modification time = "9/8/2015 1:08:51 PM"

- Modification editor = "Chris Pratt"

Delete All K-α2 Peaks:

- Modification time = "7/7/2017 2:34:56 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "18.7776"

- End position = "18.7776"

- Modification time = "7/7/2017 2:36:10 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "25.7628"

- End position = "25.7628"

- Modification time = "7/7/2017 2:36:25 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "27.3613"

- End position = "27.3613"

- Modification time = "7/7/2017 2:36:46 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "35.6909"

- End position = "35.6909"

- Modification time = "7/7/2017 2:37:09 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "43.5795"

- End position = "43.5795"

- Modification time = "7/7/2017 2:37:11 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "45.3457"

- End position = "45.3457"

- Modification time = "7/7/2017 2:37:13 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "48.7121"

- End position = "48.7121"

- Modification time = "7/7/2017 2:37:16 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "53.7317"

- End position = "53.7317"

- Modification time = "7/7/2017 2:37:18 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "60.1179"

- End position = "60.1179"

- Modification time = "7/7/2017 2:37:21 PM"

- Modification editor = "Chris Pratt"

Delete Peak(s):

- Start position = "71.9705"

- End position = "71.9705"

- Modification time = "7/7/2017 2:37:24 PM"

- Modification editor = "Chris Pratt"

Search & Match:

- Allow pattern shift = "Yes"

- Auto residue = "Yes"

- Data source = "Profile and peak list"

- Demote unmatched strong = "Yes"

- Multi phase = "No"

- Restriction set = "Default"

- Restriction = "None"

- Subset name = ""

- Match intensity = "Yes"

- Two theta shift = "0"

- Identify = "Yes"

- Max. no. of accepted patterns = "5"

- Minimum score = "50"

- Min. new lines / total lines = "60"

- Search depth = "10"

- Minimum new lines = "5"

- Minimum scale factor = "0.1"

- Intensity threshold = "0"

- Use line clustering = "Yes"

- Line cluster range = "1.5"

- Search sensitivity = "1.8"

- Use adaptive smoothing = "Yes"

- Smoothing range = "1.5"

- Threshold factor = "3"

- Modification time = "7/7/2017 2:44:00 PM"

- Modification editor = "Chris Pratt"

More items… (Bookmark 6)

More items… (Bookmark 7)

More items… (Bookmark 8)

More items… (Bookmark 9)

More items… (Bookmark 10)

More items… (Bookmark 11)

More items… (Bookmark 12)

More items… (Bookmark 13)

More items… (Bookmark 14)

More items… (Bookmark 15)