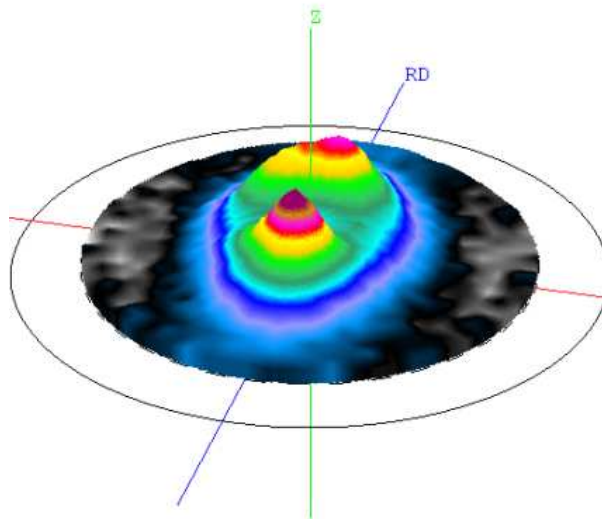




LaboTex

Version 3.0

Texture Analysis Software for Windows



LaboTex Formats

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1. Experimental Pole Figures (EPF) file format

* **EPF** (Experimental Pole Figures) files refer to the raw experimental data and their background.

In order to use the EPF files you will need a correction file: *.**COR** or *.**POW**

The table below provides a detailed description of the *. **EPF** data format:

Line	No of data in line	Description	Type
1 – 2		Arbitrary title	Character
3		Remarks for data in line 4	
4	1	Structure Code (symmetries after Schoenflies): 1 - C ₁ (triclinic) 2 - C ₂ (monoclinic) 3 - D ₂ (orthorhombic) 4 - C ₄ (tetragonal) 5 - D ₄ (tetragonal) 6 - T (cubic) 7 - O (cubic) 8 - C ₃ (trigonal) 9 - D ₃ (trigonal) 10 - C ₆ (hexagonal) 11 - D ₆ (hexagonal)	Integer
4	2	Lattice constant, a (absolute or relative)	Real
4	3	Lattice constant, b (absolute or relative)	Real
4	4	Lattice constant, c (absolute or relative)	Real
4	5	Lattice angle, α in degrees	Real
4	6	Lattice angle, β in degrees	Real
4	7	Lattice angle, γ in degrees	Real
5	1	Number of Pole Figures (including background PFs) (N)	Integer
6		Remarks for data in line 7	Character
7 to 7+N	1	2 θ Bragg angle in degrees	Real
7 to 7+N	2	α_s - beginning of polar angle in degrees	Real
7 to 7+N	3	α_e - ending of polar angle in degrees	Real
7 to 7+N	4	$\Delta\alpha$ - step of polar angle in degrees. Permissible value: 1.0, 1.2, 1.25, 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0.*	Real
7 to 7+N	5	β_s - beginning of azimuthal angle in degrees (0 or 2.5)	Real Positive values for pole figures drawn clockwise or negative values for counter-clockwise
7 to 7+N	6	β_e - ending of azimuthal angle in degrees	Real Positive values for pole figures drawn clockwise or negative values for counter-clockwise
7 to 7+N	7	$\Delta\beta$ - step of azimuthal angle in degrees . Permissible values: 1.0, 1.2, 1.25, 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0 for textured pole figures, and the same values or multiplicity of above-mentioned values for background PFs	Real Positive values for pole figures drawn clockwise or negative values for counter-clockwise
7 to 7+N	8	Index - must be 0	Real
7 to 7+N	9	Index <i>h</i> of <i>hkl</i> pole figure	Integer
7 to 7+N	10	Index <i>k</i> of <i>hkl</i> pole figure	Integer
7 to 7+N	11	Index <i>l</i> of <i>hkl</i> pole figure	Integer
7 to 7+N	12	Type of Data (1-Pole Figure, 0-Background)	Integer
7+N+1		Blank line	
7+N+2	1 to 8	Data 1 to 8 (1 st Pole Figure)	Real
7+N+3	1 to 8	Data 9 to 16 (1 st Pole Figure)	Real
7+N+4 to end of data for 1 st PF	1 to 8	Data for 1 st Pole Figure	Real
...		Blank line (separates block of data)	
...	1 to 8	Data for 2 nd pole figure	Real
...		Blank line (separates block of data)	
...	1 to 8	Data for the next PF (up to end followed by blank line)	Real

Please note: Real and integer input data must be separated by one or more space signs.

*LaboTex version 2.1.006 and higher allows new grid cell 1.8x1.8,2.25x2.5,3.6x3.6,4.5x4.5 (exceptions: trigonal,hexagonal and crystal lattice symmetry)

See the specifications below for: EPF Example, COR file format , POW file format , PPF file format , SOR file format.

2. EPF Example

Example of an experimental data file *.EPF - test.epf:

```
line 1: Test of LaboTex program - ADC method for ODF calculation.
line 2: Sample: FeSi, pole figures: 200 110 112
line 3: Structure Code a b c alfa beta gamma
line 4: 7 1 1 1 90 90 90
line 5: 6 number of Pole Figures
line 6: 2theta alf-s alf-e d-alf bet-s bet-e d-bet indx H K L P/B
line 7: 45.250 0.0 85.0 5.0 0.0 355.0 5.0 0 2 0 0 1
line 8: 52.050 0.0 85.0 5.0 0.0 355.0 5.0 0 1 1 0 1
line 9: 77.450 0.0 85.0 5.0 0.0 355.0 5.0 0 1 1 2 1
line 10: 48.500 0.0 85.0 5.0 0.0 270.0 90.0 0 2 0 0 0
line 11: 70.000 0.0 85.0 5.0 0.0 270.0 90.0 0 1 1 0 0
line 12: 80.000 0.0 85.0 5.0 0.0 270.0 90.0 0 1 1 2 0
line 13:
line 14: 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763.
line 15: 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763.
line 16: 172763. 172763. 172763. 172763. 172763. 172763. 172763. 172763.
... (line 17-172)
line 173: 12871. 15208. 15536. 13571. 10464. 7874. 6977. 7874.
line 174: 10464. 13571. 15536. 15208. 12871. 9947. 7753. 6885.
line 175: 7512. 9977. 15302. 23949. 32907. 36331. 32369. 25152.
line 176:
line 177: 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319.
line 178: 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319.
line 179: 12319. 12319. 12319. 12319. 12319. 12319. 12319. 12319.
... (line 180-335)
line 336: 11977. 13260. 15924. 19655. 23043. 23659. 22398. 23659.
line 337: 23043. 19655. 15924. 13260. 11977. 12233. 14581. 19084.
line 338: 24630. 30445. 36111. 40462. 38757. 30857. 21645. 15090.
line 339:
line 340: 142442. 142442. 142442. 142442. 142442. 142442. 142442. 142442.
line 341: 142442. 142442. 142442. 142442. 142442. 142442. 142442. 142442.
line 342: 142442. 142442. 142442. 142442. 142442. 142442. 142442. 142442.
... (line 343-498)
line 499: 19467. 17249. 16302. 15782. 15387. 15200. 15068. 15200.
line 500: 15387. 15782. 16302. 17249. 19467. 22203. 22229. 18484.
line 501: 13296. 9168. 7555. 7739. 8997. 11247. 13362. 14321.
line 502:
line 503: 830. 792. 679. 717. 830. 792. 679. 717.
line 504: 822. 784. 672. 710. 814. 777. 666. 703.
line 505: 806. 769. 659. 696. 798. 762. 653. 689.
... (line 506-508)
line 509: 519. 495. 424. 448. 441. 421. 361. 381.
line 510: 362. 346. 296. 313. 287. 274. 235. 248.
line 511: 220. 210. 180. 190. 164. 157. 134. 142.
line 512:
line 513: 2258. 2156. 1848. 1951. 2258. 2156. 1848. 1951.
line 514: 2258. 2156. 1848. 1951. 2236. 2134. 1830. 1931.
line 515: 2236. 2134. 1830. 1931. 2236. 2134. 1830. 1931.
... (line 516-518)
line 519: 1981. 1891. 1621. 1711. 1851. 1767. 1515. 1599.
line 520: 1637. 1562. 1339. 1413. 1329. 1268. 1087. 1147.
line 521: 922. 880. 754. 796. 330. 315. 270. 285.
line 522:
line 523: 9209. 8791. 7535. 7954. 9209. 8791. 7535. 7954.
line 524: 9118. 8704. 7460. 7875. 9118. 8704. 7460. 7875.
line 525: 9029. 8618. 7387. 7798. 8941. 8535. 7315. 7722.
... (line 526-528)
line 529: 7611. 7265. 6227. 6573. 6977. 6660. 5708. 6025.
line 530: 5903. 5635. 4830. 5098. 4723. 4508. 3864. 4079.
line 540: 3143. 3000. 2572. 2715. 1246. 1190. 1020. 1076.
```

See the specifications below for: EPF file format, COR file format, POW file format, PPF file format, SOR file format.

3. PPF file format

***PPF** (Preliminary Corrected Pole Figures^K) files refer to the experimental data after conducting the background and de-focussing effects corrections using external procedures (not conducted in LaboTex).

The structure of a ***PPF** file is identical to ***EPF** and ***POW** except for the data for the background of pole figures.

See the specifications below for: EPF file format, COR file format, POW file format , SOR file format .

4. SOR file format

***SOR** (Single Orientation) files refer to experimental, single orientation set in the LaboTex format

The table below provides a detailed description of ***SOR** data format:

Line	No of data in line	Description	Type
1 - 2		Arbitrary title	Character
3		Remarks for data in line 4	
4	1	Structure Code (symmetries after Schoenflies): 1 - C ₁ (triclinic) 2 - C ₂ (monoclinic) 3 - D ₂ (orthorhombic) 4 - C ₄ (tetragonal) 5 - D ₄ (tetragonal) 6 - T (cubic) 7 - O (cubic) 8 - C ₃ (trigonal) 9 - D ₃ (trigonal) 10 - C ₆ (hexagonal) 11 - D ₆ (hexagonal)	Integer
4	2	Lattice constant, a (absolute or relative)	Real
4	3	Lattice constant, b (absolute or relative)	Real
4	4	Lattice constant, c (absolute or relative)	Real
4	5	Lattice angle, α in degrees	Real
4	6	Lattice angle, β in degrees	Real
4	7	Lattice angle, γ in degrees	Real
4	8	Step for output ODF (grid cells). Permissible values (deg): 1.0, 1.2, 1.25, 1.5, 2.0, 2.5, 3.0, 3.75, 5.0, 6.0, 7.5, 10.0*	Real
4	9	Weight for data (1 – present, 0 – absent)	Integer
4	10	Angle Unit: 0 – deg, 1 – rad	Integer
4	11	Angle Convention: 0 – Bunge 1 – Roe	Integer
5 to the end	1	ϕ_1	Real
5 to the end	2	Φ	Real
5 to the end	3	ϕ_2	Real
5 to the end	[4]	Weight (optionally) (if parameter <i>weight</i> in line 4 is 1)	Real

Note: Real and integer input data must be separated in line by one or more spaces.

*LaboTex allows new grid cell from version 21.006: 1.8x1.8,2.25x2.5,3.6x3.6,4.5x4.5 (exceptions: trigonal,hexagonal crystal lattice symmetry

See the specifications below for: EPF file format, COR file format, POW file format , PPF file format.

5. POW format

*.**POW** (**POW**der pole figures) files refer to the powder sample pole figures measured, if possible, for a specific sample.

You should measure the pole figures of the powder sample for defocusing correction from the same material as the "textured samples". The powder sample is treated as "non-texture" sample which helps to identify the absorption curve for defocusing correction.

The structure of *. **POW** file is identical to *.**EPF**.

See the specifications below for: EPF file format, COR file format, SOR file format , PPF file format.

6. COR format

*.**COR** (**COR**rection) files refer to coefficients for the de-focussing effect.

*.**COR** files contain a set of correction coefficients for the de-focussing effect.

The table below provides a detailed description of *.**COR** data format:

Line	No of data in line	Description	Type
1 – 2		Arbitrary title	Character
3	1 to n	α in degrees (polar angle)	Real
4	1	{hkl} of first pole figure (three digits number)	Real
4	2 to n+1	correction coefficients for de-focussing effect	Real
5	1	{hkl} of second pole figure (three digits number)	Real
5	2 to n+1	correction coefficients for de-focussing effect	Real
...		...	
3+N*2	1	{hkl} (three digits number) N - number of pole figure	Real
4+N*2	2 to n+1	correction coefficients for de-focussing effect	Real

Please note: Real and integer input data must be separated by one or more space signs.

See the specifications below for : EPF file format, PPF file format, SOR file format, POW file format.

7. Other formats

List of the compatible LaboTex data formats:

(For the updates and the current list of LaboTex compatible file formats see : www.labosoft.com.pl/format.htm)

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- **'TSV'** Single Orientations Files,
 - Single orientations data files: *.tsv can be selected from *File->New Sample-> Choose Experimental Data*
- **'PLF'** Queens Univ. PF Format files (4*5deg) - (corrected pole figures),
 - Pole figures data files : *.plf can be selected from *File->New Sample-> Choose Experimental Data*
- **'PLF'** 5*5deg - (corrected pole figures),
 - Pole figures data files : *.plf can be selected from *File->New Sample-> Choose Experimental Data*
- **'CON'** McGill University PF Format files - (corrected pole figures),
 - Pole figures data files : *.con can be selected from *File->New Sample-> Choose Experimental Data*

- 'HKL' HKL - Kawasaki KTEC Format files - (corrected pole figures),
 - Pole figures data files : *-hkl. can be selected from *File->New Sample-> Choose Experimental Data*
- 'hkl' AGH main format,
 - Pole figures data files : *.hkl can be selected from *File->New Sample-> Choose Experimental Data*
 - Background pole figures data files: *-b.hkl can be selected from *File->New Sample-> Choose Experimental Data*
 - Random(powder) pole figures data files: *-p.hkl can be selected from *File->New Sample-> Choose Experimental Data*
 - Background random(powder) pole figures data files: *-t.hkl can be selected from *File->New Sample-> Choose Experimental Data*
- 'xfb' AGH second format (corrected pole figures),
 - Pole figures data files : *.xfb can be selected from *File->New Sample-> Choose Experimental Data*
- 'CTF' HKL Single Orientations Files,
 - Single orientations data files: *.CTF can be selected from *File->New Sample-> Choose Experimental Data*
- 'SNG' TSL Single Orientations Files,
 - Single orientations data files: *.sng can be selected from *File->New Sample-> Choose Experimental Data*
- 'TXT' HKL Single Orientations Files,
 - Single orientations data files: *.txt can be selected from *File->New Sample-> Choose Experimental Data*
- 'UXD' (file version 1) - SIEMENS/BRUKER (corrected pole figures, ASCII-files!,GADDS/D-8 Discover XRD). Use only one pole figure in one file. Parameter "_sample" has to contain Miller indices of PF (in triangle brackets), for example: "Ir<111>".
 - Pole figures data files: *.uxd can be selected from *File->New Sample-> Choose Experimental Data*
 - **Please note:** Convert the binary files from the GADDS/D-8 Discover XRD to the the ASCII UXD files using software from Siemens/Bruker (XCH or other).
- 'UXD' (file version 2) - BRUKER (corrected pole figures, ASCII-file!,GADDS/D-8 Discover XRD). Use only one pole figure in one file. Parameter "_sample" has to contain Miller indices of PF (in triangle brackets) for example: "Ir<111>".
 - Pole figures data files: *.uxd can be selected from *File->New Sample-> Choose Experimental Data*
 - **Please note:** Convert the binary files from the GADDS/D-8 Discover XRD to the the ASCII UXD files using software from Bruker (XCH or other).
LaboTex can read background files for UXD format:

1) please mark the data for background with a 'B' letter in the indices of the pole figure (within the filename, for example '<111B>cu brut').

```

-----
_FILEVERSION=2
_SAMPLE="<111B> cu brut"
_SITE='UNIV ...'
_USER='LAMBDA'
...
-----

```

2) LaboTex requires one pole figure on one *.UXD file.

Each pole figure and background file has to be in a separate file with an extension *.UXD.

For examples use the following naming system: sample_100.UXD, sample_100BL.UXD, sample_100BR.UXD,

...

The files with names terminating with BL or BR are background from the 'left' and 'right' side of PF; LaboTex average BL and BR values are used.

3) You may choose to use only BL or BR files.

4) Background files in the *.UXD format are only allowed for one background value of one alpha value!

For a pole figure called, for example, Cu-brut_111.UXD, create 3 files in XRD software:

a) Cu-brut_111.UXD (pole figure data+ parameter sample: _SAMPLE="<111> cu brut")

b) Cu-brut_111BL.UXD (left background data + parameter sample: _SAMPLE="<111B> cu brut")

c) Cu-brut_111BR.UXD (right background data+ parameter sample: _SAMPLE="<111B> cu brut")

- 'UXD' Similarly to 'UXD' formats above (SIEMENS/BRUKER file version 1 and 2) use it only with reversed radial direction! Remember to correct the pole figures converting them to ASCII-files.
- 'HKL' Chalk River Neutron Diffr. Data (corrected pole figures)
 - Pole figures data files: *.* can be selected from *File->New Sample-> Choose Experimental Data*
- 'ANA' - EMSE Format files (corrected pole figures)
 - Pole figures data files: *.ana can be selected from *File->New Sample-> Choose Experimental Data*
- 'epf' - popLA PF Format files (corrected pole figures).

Warning: Files in popLA format have the same extension as LaboTex files: "EPF"! For files in popLA select format "epf" (**small capitals!**) in LaboTex Options.

- Pole figures data files: *.epf can be selected from *File->New Sample-> Choose Experimental Data*
- 'RAW' - popLA Format files
 - Pole figures data files: *.raw can be selected from *File->New Sample-> Choose Experimental Data*
 - Defocusing correction data files: *.dfb can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'ASC' - Rigaku ASC format (1PF/file)
 - Pole figures data files: *.asc can be selected from *File->New Sample-> Choose Experimental Data*
 - Random (powder) pole figures data files: : *.asc can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'XPF' - BEARTEX data format (corrected pole figures)
 - Pole figures data files: *.xpf can be selected from *File->New Sample-> Choose Experimental Data*
- 'PFG' - RIST data format from RIGAKU (ASCII)
 - Pole figures data files: *.pfg can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.pfg can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'TXT' - RIST data format from PHILIPS (ASCII- corrected pole figures)
 - Pole figures data files: *.txt can be selected from *File->New Sample-> Choose Experimental Data*
- 'RW1' - PHILIPS X'Pert binary data format (Binary)

- Pole figures data files: *.rw1 can be selected from *File->New Sample-> Choose Experimental Data*
 - Background pole figures data files: *.bgr can be selected from *File->New Sample-> Choose Experimental Data*
 - Defocusing correction data files: *.cor can be selected from *File->New Sample-> Choose Defocussing Correction*
- Please note:** Background pole figures data files can have the same extension as defocusing correction data files ('COR'). Please change the 'COR' extension for background files to 'BGR'!
- **'NJA'** - Seifert ASCII data format (compatible also with data from PSD)
 - Pole figures data files: *.NJA can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.NJA can be selected from *File->New Sample Choose Defocussing Correction*
 - **'NJC'** - Seifert binary data format (compatible also with the data from PSD)
 - Pole figures data files: *.NJC can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.NJC can be selected from *File->New Sample-> Choose Defocussing Correction*
 - **'DAT'** - Seifert ISO-DEBYFLEX 3003 - ASCII data format. Use only one pole figure in one file. Pole figure indices are 3 last characters before point in file name (example: PC_200.DAT for 200 pole figure). Optionally you may add the parameter "2THETA" before label "XDATA" in file (for example 2THETA=33.45). Values of 2THETA are essential for defocusing correction from Schultz equation. You may also use the non-equal angle step: 5deg for the inclination angle (chi or alpha) and 10 deg for the azimuthal angle (phi or betha) – the data are approximated to 5x5 grid. The background data (one data for each value of the inclination angle) are positioned first after label "XDATA".
 - Pole figures data files: *.DAT can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.DAT can be selected from *File->New Sample-> Choose Defocussing Correction*
 - **'COA'** COA data format (corrected pole figures).
 - **'POL'** - The University of Birmingham/HiltonBrooks Texture Data.
 - Pole figures data files: *.POL can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.POL can be selected from *File->New Sample-> Choose Defocussing Correction*
 - **'DAT'** - TU Berlin data format (1PF/file)
 - Pole figures data files: *.DAT can be selected from *File->New Sample-> Choose Experimental Data*
 - **'POL'** - The University of Birmingham with background (add '_b' to filename for background data).
 - Pole figures data files: *.POL can be selected from *File->New Sample-> Choose Experimental Data*
 - Background data for pole figures (filename_b.pol): *.POL can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.POL can be selected from *File->New Sample-> Choose Defocussing Correction*
 - Background data for random pole figures (filename_b.pol): *.POL *File->New Sample-> Choose Defocussing Correction*
 - **'000'** - U.Paris-Sud (Neutron Diffr.Data) (1PF/file) (add '_b' to filename for background data)
 - Pole figures data files: *.DAT can be selected from *File->New Sample-> Choose Experimental Data*

- Background data for pole figures (filename_b.000): *.DAT can be selected from *File->New Sample-> Choose Experimental Data*
- 'RWA' - Philips ATC3 (add '_b' to filename for background data)
 - Pole figures data files: *.RWA can be selected from *File->New Sample-> Choose Experimental Data*
 - Background data for pole figures (filename_b.RWA): *.RWA can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.RWA can be selected from *File->New Sample-> Choose Defocussing Correction*
 - Background data for random pole figures (filename_b.RWA): *.RWA can be selected from *File->New Sample-> Choose Defocussing Correction*
- 'M' - University of Northeastern (Shenyang) (add '_b' to filename for background data)
 - Pole figures data files: *.M can be selected from *File->New Sample-> Choose Experimental Data*
 - Background data for pole figures (filename_b.M): *.M can be selected from *File->New Sample-> Choose Experimental Data*
 - Random pole figures data files: *.M can be selected from *File->New Sample-> Choose Defocussing Correction*
 - Background data for random pole figures (filename_b.M): *.M can be selected from *File->New Sample-> Choose Defocussing Correction*

In order to create non-LaboTex file format accessible for creation of CPF objects:

- a) select 'Edit' from the main LaboTex menu;
- b) select 'LaboTex Options'
- c) select the tab 'Data Formats'
- d) select the name for format from the drop down list in the positions 4 -7

You may use several files simultaneously:

select 'File'>'New Sample' from the main LaboTex menu and then holding the 'Ctrl' key click the desired files in the file list.

If your file extensions differ from the ones listed in this document, please change them accordingly. For example, in the RW1 format the background pole figures the data files have a default *.COR extension and this extension is the same as the one for defocusing correction data files. To avoid confusion, change the extension of background pole figures data files to *.BGR before you include them in LaboTex.