

LaboTex Formats

1. EPF file format

It needs correction file: **COR** or **POW**

Experimental Pole Figures, i.e. raw experimental data and their background.

Description of *filename.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

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 also: EPF Example, COR file format , POW file format , PPF file format , SOR file format.

2. EPF Example

Example of experimental data file type *filename.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 also: EPF file format, COR file format, POW file format, PPF file format, SOR file format.

3. PPF file format

filename.PPF - Preliminary Corrected Pole Figures^K i.e. experimental data after the background and defocussing effects corrections using procedures external to LaboTex program.

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

See also: EPF file format, COR file format, POW file format, SOR file format.

4. SOR file format

filename.SOR – Single ORientation File i.e. experimental, single orientation set in LaboTex format

Description of *filename.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 also: EPF file format, COR file format, POW file format, PPF file format.

5 POW format

filename.POW - POWder 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 help to find out the absorption curve for defocusing correction.

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

See also: EPF file format, COR file format, SOR file format, PPF file format.

6. COR format

filename.COR - CORrection coefficients for the de-focussing effect.

File contains set of correction coefficients for the de-focussing effect.

Description of *filename.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

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

See also: EPF file format, PPF file format, SOR file format, POW file format.

7. Other formats

For current list of LaboTex compatible formats see : <http://www.labosoft.com.pl/format.htm>

List of the compatible LaboTex data formats:

All trademarks are the properties of their respective owners and are only used in a descriptive fashion without any intention to infringe.

- **'TSV'** Single Orientations Files,
 - Single orientations data files: *.tsv (input from "Choose Experimental Data" list)
- **'PLF'** Queens Univ. PF Format files (4*5deg) - (corrected pole figures),
 - Pole figures data files : *.plf (input from "Choose Experimental Data" list)
- **'PLF'** 5*5deg - (corrected pole figures),
 - Pole figures data files : *.plf (input from "Choose Experimental Data" list)
- **'CON'** McGill University PF Format files - (corrected pole figures),
 - Pole figures data files : *.con (input from "Choose Experimental Data" list)
- **'HKL'** HKL - Kawasaki KTEC Format files - (corrected pole figures),
 - Pole figures data files : *-hkl. (input from "Choose Experimental Data" list)
- **'hkl'** AGH main format,
 - Pole figures data files : *.hkl (input from "Choose Experimental Data" list)
 - Background pole figures data files: *-b.hkl (input from "Choose Experimental Data" list)
 - Random(powder) pole figures data files: *-p.hkl (input from "Choose Experimental Data" list)
 - Background random(powder) pole figures data files: *-t.hkl (input from "Choose Experimental Data" list)

- 'xfb' AGH second format (corrected pole figures),
 - Pole figures data files : *.xfb (input from "Choose Experimental Data" list)
- 'CTF' HKL Single Orientations Files,
 - Single orientations data files: *.CTF (input from "Choose Experimental Data" list)
- 'SNG' TSL Single Orientations Files,
 - Single orientations data files: *.sng (input from "Choose Experimental Data" list)
- 'TXT' HKL Single Orientations Files,
 - Single orientations data files: *.txt (input from "Choose Experimental Data" list)
- '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 (input from "Choose Experimental Data" list)
 - **Notice:** 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 (input from "Choose Experimental Data" list)
 - **Notice:** 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) data for background please mark with 'B' letter in indices of pole figure (in filename - for example '<111B>cu brut').

```

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

 - 2) LaboTex requires one pole figure on the one UXD file.
 Each pole figure and background file has to be in separate file with extension UXD.
 For example: sample_100.UXD, sample_100BL.UXD, sample_100BR.UXD, ...
 (files with terminations BL or BR are background from 'left' and 'right' side of PF.
 LaboTex average BL and BR values).
 - 3) You may use only BL or BR file, too.
 - 4) Background files in UXD format are allowed only one background value for one alpha value!
 In case one pole figure called for example Cu-brut_111.UXD you should make 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' As 'UXD' formats above (SIEMENS/BRUKER file version 1 and 2) - only with reversed radial direction! Corrected pole figures (ASCII-files).
- 'HKL' Chalk River Neutron Diffraction Data (corrected pole figures)

- Pole figures data files: *.* (input from "Choose Experimental Data" list)
- 'ANA' - EMSE Format files (corrected pole figures)
 - Pole figures data files: *.ana (input from "Choose Experimental Data" list)
- 'epf' - popLA PF Format files (corrected pole figures). Warning: Files in popLA format have the same extension as LaboTex files: "EPF". Select "epf" (small letter!!!) data format in LaboTex Options for files in popLA format.
 - Pole figures data files: *.epf (input from "Choose Experimental Data" list)
- 'RAW' - popLA Format files
 - Pole figures data files: *.raw (input from "Choose Experimental Data" list)
 - Defocusing correction data files: *.dfb (input from "Choose Defocusing Correction" list)
- 'ASC' - Rigaku ASC format (1PF/file)
 - Pole figures data files: *.asc (input from "Choose Experimental Data" list)
 - Random(powder) pole figures data files: : *.asc (input from "Choose Defocusing Correction" list)
- 'XPF' - BEARTEX data format (corrected pole figures)
 - Pole figures data files: *.xpf (input from "Choose Experimental Data" list)
- 'PFG' - RIST data format from RIGAKU (ASCII)
 - Pole figures data files: *.pfg (input from "Choose Experimental Data" list)
 - Random pole figures data files: *.pfg (input from "Choose Defocusing Correction" list)
- 'TXT' - RIST data format from PHILIPS (ASCII- corrected pole figures)
 - Pole figures data files: *.txt (input from "Choose Experimental Data" list)
- 'RW1' - PHILIPS X'Pert binary data format (Binary)
 - Pole figures data files: *.rw1 (input from "Choose Experimental Data" list)
 - Background pole figures data files: *.bgr (input from "Choose Experimental Data" list)
 - Defocusing correction data files: *.cor (input from "Choose Defocusing Correction" list)

Warning: Background pole figures data files can have the same extension as defocusing correction data files ('COR'). Please change 'COR' extension of background files to 'BGR'!
- 'NJA' - Seifert ASCII data format (compatible also with data from PSD)
 - Pole figures data files: *.NJA (input from "Choose Experimental Data" list)
 - Random pole figures data files: *.NJA (input from "Choose Defocusing Correction" list)
- 'NJC' - Seifert binary data format (compatible also with data from PSD)
 - Pole figures data files: *.NJC (input from "Choose Experimental Data" list)
 - Random pole figures data files: *.NJC (input from "Choose Defocusing Correction" list)
- '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 non equal angle step: 5deg for inclination angle (chi or alpha) and 10 deg for the

azimuthal angle (phi or betha) - data are approximated to 5x5 grid. Background data (one data for each value of inclination angle) are first after label "XDATA".

- Pole figures data files: *.DAT (input from "Choose Experimental Data" list)
- Random pole figures data files: *.DAT (input from "Choose Defocusing Correction" list)
- 'COA' COA data format (corrected pole figures).
- 'POL' - The University of Birmingham/HiltonBrooks Texture Data.
 - Pole figures data files: *.POL (input from "Choose Experimental Data" list)
 - Random pole figures data files: *.POL (input from "Choose Defocusing Correction" list)
- 'DAT' - TU Berlin data format (1PF/file)
 - Pole figures data files: *.DAT (input from "Choose Experimental Data" list)
- 'POL' - The University of Birmingham with background (add '_b' to filename for background data).
 - Pole figures data files: *.POL (input from "Choose Experimental Data" list)
 - Background data for pole figures (filename_b.pol): *.POL (input from "Choose Experimental Data" list)
 - Random pole figures data files: *.POL (input from "Choose Defocusing Correction" list)
 - Background data for random pole figures (filename_b.pol): *.POL (input from "Choose Defocusing Correction" list)
- '000' - U.Paris-Sud (Neutron Difr.Data) (1PF/file) (add '_b' to filename for background data)
 - Pole figures data files: *.DAT (input from "Choose Experimental Data" list)
 - Background data for pole figures (filename_b.000): *.DAT (input from "Choose Experimental Data" list)
- 'RWA' - Philips ATC3 (add '_b' to filename for background data)
 - Pole figures data files: *.RWA (input from "Choose Experimental Data" list)
 - Background data for pole figures (filename_b.RWA): *.RWA (input from "Choose Experimental Data" list)
 - Random pole figures data files: *.RWA (input from "Choose Defocusing Correction" list)
 - Background data for random pole figures (filename_b.RWA): *.RWA (input from "Choose Defocusing Correction" list)
- 'M' - University of Northeastern (Shenyang) (add '_b' to filename for background data)
 - Pole figures data files: *.M (input from "Choose Experimental Data" list)
 - Background data for pole figures (filename_b.M): *.M (input from "Choose Experimental Data" list)
 - Random pole figures data files: *.M (input from "Choose Defocusing Correction" list)
 - Background data for random pole figures (filename_b.M): *.M (input from "Choose Defocusing Correction" list)
-

To make non-LaboTex format accessible for creation of CPF objects you should:

- a) select EDIT menu in LaboTex
- b) select LaboTex Options

- c) select Data Formats
- d) select name of format from selection windows 4 -7

You may use several files simultaneously:

in "New Sample" dialog box select (click mouse) several files simultaneously holding CTRL (control) key.

If extensions of files with data differ from higher indicated please to change it.
For example: (case RW1 format) background pole figures data files have a COR extension as default which is the same as defocusing correction data files. Change extension of background pole figures data files to BGR before input to LaboTex.