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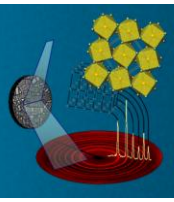
Fundamentals of Powder Diffraction and Structural Characterization of Materials
Second Edition



pks2ind conversion utility

The program *pks2ind* converts any ASCII table into ITO, TREOR and DICVOL formats. By default, the following input data file (free format within each row) is assumed:

```
 45401      53   10.1309    0.0001  0.073  0.001  0.675  -0.002  0.058
111415     175   13.1251    0.0001  0.068  0.001  0.663  -0.001  0.044
321660     447   15.3441    0.0001  0.069  0.001  0.663  -0.001  0.044
…
```

- **1st column – integrated intensity**;
- 2nd column – error for intensity;
- **3rd column – peak position in degrees 2θ**;
- 4th column – error in peak position;
- 5th column – full width at half maximum in degrees;
- 6th column – mixing parameter (pseudo-Voigt) or exponent (Pearson-VII);
- 7th column – peak asymmetry;
- 8th column – R_p.

Default file extension is .pks; other formats of data can be converted, as long as at least one column in the file corresponds to observed Bragg angles. The presence of observed integrated intensities is optional. The last row in the data file must be empty. No comment row(s) are allowed. Numbers in each row must be separated by at least one space or by commas.

User input:

1) Enter sample shift in mm:

- Type the sample displacement from the optical axis of the goniometer (in mm assuming goniometer radius 250 mm), if known. Default = 0 (no sample displacement correction). Sample displacement can be established by using internal standard data or a certain average value from previous experiments, where the specimen preparation was nearly identical. Random sample displacements can be introduced, usually in the range from –0.2 mm to 0.2 mm with a step 0.05 mm, if previous *ab-initio* indexing attempts using all three indexing programs failed.

2) Enter columns # for 2theta & intensity [3,1]:

- For the standard file format (see above), accept the defaults (press ENTER);
- For any another file format, enter column numbers for 2θ (required) and intensity (optional) and press ENTER.

Program output:

- The program generates three files with extentions ".ito", ".tre", and ".dic" for ITO, TREOR and DICVOL programs, respectively, using the most common defaults for variables, for example: Cu Kα radiation, indexing cubic through orthorombic system (TREOR), etc. When necessary the resultant files may be edited using a suitable ASCII editor (e.g., notepad).

Example:

Consider the file **Ch14Ex01_CuKa.pks** found online http://www.springer.com/978-0-387-09578-3. It contains the following information:

```
Sample          LaNi4.85Sn0.15
Comment1        Powder indexing example No.1. Peak list. (Chapter 14)
Comment2        Cu K radiation
Copyright       (C) Springer 2009
-----     --------     ----------
I/I0      2T (deg)     FWHM (deg)
-----     --------     ----------
20        20.288       0.070
43        22.105       0.077
513       30.198       0.076
305       35.548       0.078
…
55        81.632       0.175
```

Before employing it as the input file for *pks2ind*, it should be edited and the first 7 lines (comments) should be removed. Thus, the input file (**Copy of Ch14Ex01_CuKa.pks**) has been converted into

```
20        20.288       0.070
43        22.105       0.077
513       30.198       0.076
305       35.548       0.078
…
55        81.632       0.175
```

Bragg angles are in column 2, and intensities are in column 1. The *pks2ind* utility can be started in a separate DOS window, or the file to be converted can simply be dragged and dropped into the icon on the desktop containing a shortcut to *pks2ind* as shown in Figure 1, below.

Figure 1. Starting the *pks2ind* utility by dragging and dropping the **Copy of Ch14Ex01_CuKa.pks** file on the icon representing a desktop shortcut to *pks2ind*.

The dialog is shown in Figure 2.

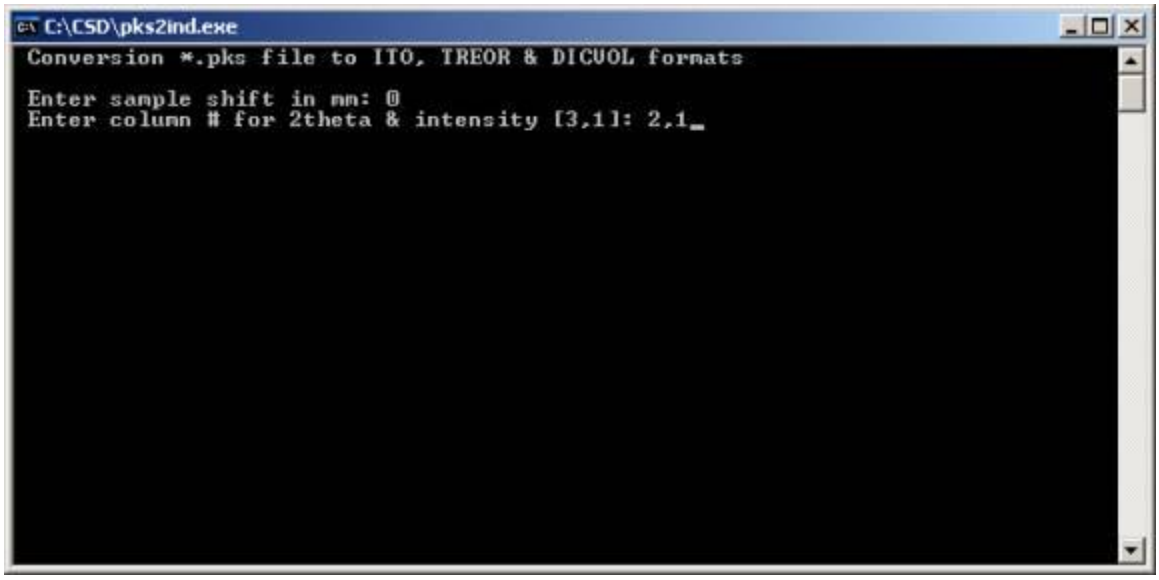


Figure 2. The dialog in the *pks2ind* utility specifying no sample displacement correction of the data and identifying columns 2 and 1 as those that contain Bragg angles and intensities, respectively.

The resultant output files are shown below.

```
C:\Full path      Sample displacement correction   # of observed peaks.
 24 2 1 1 1 1 1 0
25. 25. 25. 10. 1500. 90. 130.
1.54056 0. 0. 0.
0.03 0.
 20.288
 22.105
 30.198
 35.548
 …
 81.632
```

Figure 3. Input file for DICVOL (**Copy of Ch14Ex01_CuKa.dic**) produced by *pks2ind*.

```
C:\Full path      Sample displacement correction   # of observed peaks.
9018 0 0 0  3.0  3.5   1.54060 011 3 6 6 6 0 0 1 0              4.0
     0.000        4.0       14
 20.28814  22.10520  30.19870  35.54854  41.28562  42.27299  44.21113  45.13051
 47.33229  49.965 6  51.517 9  55.621 7  58.74236  60.58438  62.82445  63.86623
 68.48545  74.05018  74.353 8  75.29838  78.958 6  79.629 9  81.35734  81.63223
0
END
```

Figure 4. Input file for ITO (**Copy of Ch14Ex01_CuKa.ito**) produced by *pks2ind*.

```
C:\Full path       Sample displacement correction   # of observed peaks.
       20.288              199
       22.105              429
       30.198             5129
       35.548             3049
       …
       81.632              549

CHOICE=3, VOL=1500, CEM=25, WAVE=1.54056,
END*
```

Figure 4. Input file for TREOR (**Copy of Ch14Ex01_CuKa.tre**) produced by *pks2ind*.

The title (first) line in each created file contains full path and filename, the introduced sample displacement correction, and the total number of existing Bragg peaks. The *pks2ind* utility outputs all three files into the same folder, which contains the original input file. The file names are identical to the input file name (**Copy of Ch14Ex01_CuKa**).