SHORT DESCRIPTION OF Ind_X 1.0 October 19, 2016

Function: Ind_X 1.0 is a program for indexing diffraction data given in the form of reciprocal lattice nodes.

Operating system: MS Windows

Language: Fortran 90

Distribution: Free for academic use.

Method: See a paper on this subject at `http://imim.pl/personal/adam.morawiec`.

Execution: Run `Ind_X` and respond to the question about filename, or run `Ind_X filename.idx`. The filename must **not** contain spaces; otherwise, use `Ind_X "filename with spaces.idx"`. The extension .idx is mandatory.

Input file: To learn the structure of the input file examine example.ipx. The input file contains keywords followed by appropriate data. Some keywords are mandatory. The file must contain the keyword `_NumberOfReflections` followed by a line specifying the number of reflections to be used. The number of reflections must be in the range $[4, 999]$. For instance, with 26 reflections, one will have

```
_NumberOfReflections
       26
```

Then, the file must contain the reflections (nodes of the reciprocal lattice) specified by their Cartesian coordinates

```
_Reflections
    -0.0082128   0.0682666  -0.0729906
    -0.0490259   0.2322427  -0.0700842
         ...        ...        ...
```

Alternatively, the reflections can be specified by angles θ, φ and χ of classic Eulerian goniostat

```
_Wavelength
   1.54056
_ReflectionsThetaPhiChi
   4.43    6.86  -46.71
  10.99   11.92  -16.45
    ...      ...     ...
```

or by the angles θ, φ and κ of kappa goniometer

```
_Wavelength
   1.54056
_AngleOfKappaAxis
    50.0
_ReflectionsThetaPhiKappa
     -16.81328   -14.38328   -62.32923
       4.02345     4.95345   -21.52666
    ...      ...     ...
```

The parameter(s) `_Wavelength` (and `_AngleOfKappaAxis`) must precede `_ReflectionsThetaPhiChi` (and, respectively, `_ReflectionsThetaPhiKappa`). The conversion between the angles (θ, φ, χ) and (θ, φ, κ) is the same as that at `http://7id.xray.aps.anl.gov/calculators/kappa.html`. The relationship between coordinates of reciprocal lattice vectors and (θ, φ, χ) are the same as in [A.J.M. Duisenberg, *J. Appl. Cryst.* **25**, 92–96 (1992)].

In principle, the computation is unit-independent but the input-output formats are intended for Ångström [Å] as a unit of length. The angles must be in degrees.

The list of optional keywords includes:

	Type	Range	Default
_MinMaxVolumeOfPrimitiveCell	F F	> 0.0	
_TypeOfPeriodogram	I	$[-3, 3]$	0
_UserProvidedTestVolumes	I FF...F	$n \in [1, 350]$, $r > 0.0$	
_MaxAllowedMillerIndex	I	$[4, 100]$	100
_TheMainCriterion	F	$[0.03, 0.30]$	0.12
_WeightsForSortingBases	F F	> 0.0	0.3 0.7
_FractionOfSupportingReflections	F	$(0.0, 1.0]$	$\min(12.0/N,\ 0.5)$
_ExtentOfTheSearch	I	$\{1, 2, 3\}$	2
_MaxNumberOfSavedBases	I	$[1, 128]$	16
_SortSolutionsByQualityVsVolume	I	$\{0, 1, 2, 3\}$	0
_SaveLePage	I	$[0, 128]$	0
_CreateLogFile	I	$\{0, 1\}$	0

The symbol N denotes _NumberOfReflections.

• The keyword _MinMaxVolumeOfPrimitiveCell must be followed by a line with the smallest and the largest expected volumes of the primitive cell. For instance, assuming that the length is given in Å, the specification

```
_MinMaxVolumeOfPrimitiveCell
     100.0 100000.0
```

means that the volume of the primitive cell is assumed to be larger than 100Å^3 and smaller than 100000Å^3. The first entry must be positive, and the second must be at least 1.5 times larger than the first. _MinMaxVolumeOfPrimitiveCell is not a strict constraint, i.e., the output file may contain solutions with volumes beyond user-specified bounds. The default lower and upper bounds on the volume are, respectively, $1/r^3$ and $10000/r^3$, where r is the magnitude of the shortest among _Reflections.

• The keyword _TypeOfPeriodogram must be followed by a line with an integer indicating the type of periodogram used for getting test volumes of the primitive cell. For instance, one may have

```
_TypeOfPeriodogram
     3
```

The allowed integers are:
0 – the type of periodogram will be selected automatically (based on _ExtentOfTheSearch),
1 – periodogram obtained by epoch folding,
2 – Rayleigh periodogram,
3 – Scargle periodogram.
If the integers are negative (-1,-2 or -3), the program will stop after saving the corresponding periodogram in Ind_X_Periodogram.txt. The default value of _TypeOfPeriodogram is 0.

• The keyword _UserProvidedTestVolumes must be followed by a line with a positive integer specifying the number of user-provided test volumes of the primitive cell and by the test volumes. For instance, assuming that the length is given in Å, the specification

```
_UserProvidedTestVolumes
  3  1960.0  3032.0  5531.3
```

means that the user wants to test three volumes: 1960.0Å^3, 3032.0Å^3 and 5531.3Å^3. The number of user-provided test volumes cannot exceed 350.

• The keyword _MaxAllowedMillerIndex must be followed by a line with an integer in the range [4,100] specifying the upper bound on absolute values of Miller indices. For instance,

```
_MaxAllowedMillerIndex
     35
```

means that the absolute values of Miller indices will not exceed 35. _MaxAllowedMillerIndex is not a strict constraint, i.e., the output file may contain solutions with values beyond the user-specified bound. The default value of _MaxAllowedMillerIndex is 100.

• The keyword _TheMainCriterion must be followed by a line with a single real number in the range [0.03,0.30] specifying the allowed deviations from integer values of Miller indices. For instance,

```
_TheMainCriterion
     0.16
```

means that the allowed deviations from integer values of Miller indices cannot exceed 0.16. Reflections with such deviations are marked in output files by H- or -h. Those with deviations not exceeding half of the specified value (0.08 in the above example) are marked by H-. The default value of _TheMainCriterion is 0.12.

• The keyword _WeightsForSortingBases must be followed by a line with two non-negative real numbers specifying weights for quantifying quality of solutions. For instance,

```
_WeightsForSortingBases
     0.2  0.8
```

means that the number N_H of reflections of type H- will be taken with weight $w_H = 0.2$ and the total number N_h of reflections of types H- and -h will be taken with weight $w_h = 0.8$. The default values of _WeightsForSortingBases are $w_H = 0.3$ and $w_h = 0.7$.

• The keyword _FractionOfSupportingReflections must be followed by a line with a single positive real number not exceeding 1. The integer nearest to _FractionOfSupportingReflections × _NumberOfReflections represents the number of best reflections which will constitute the starting point of the search for the solution. For instance, with

```
_FractionOfSupportingReflections
     0.6
```

and _NumberOfReflections equal to 20, the program will look for $0.6 \times 20 = 12$ best reflections supporting a given test volume, and these reflections will be used to built a basis of the reciprocal lattice. The default value of _FractionOfSupportingReflections is $\min(12.0/N, 0.5)$.

• The keyword _ExtentOfTheSearch must be followed by a line with an integer 1, 2 or 3 specifying the extent and density of the search for the solution. E.g., one may have

```
_ExtentOfTheSearch
     3
```

The single entity _ExtentOfTheSearch controls a number of secondary program parameters. In particular, _ExtentOfTheSearch determines the density of arguments of the periodogram and the number of automatically determined test volumes. For each test volume, some extra volumes in its vicinity are also tested, and _ExtentOfTheSearch determines the number and spread of these extra volumes. The larger the value of _ExtentOfTheSearch the wider the extent of the search. The default value of _ExtentOfTheSearch is 2.

• The keyword _MaxNumberOfSavedBases must be followed by a line with an integer in the range [1,128] specifying the upper bound on the number of solutions saved in the output file. For instance,

```
_MaxNumberOfSavedBases
     50
```

means that at most 50 solutions will be saved. The default value of _MaxNumberOfSavedBases is 16.

• The keyword _SortSolutionsByQualityVsVolume must be followed by a line with an integer indicating the method of sorting solutions in the output file. For instance, one may have

```
_SortSolutionsByQualityVsVolume
     2
```

The allowed integers are:
0 – sorting by quality of solution,
1 – sorting by volume of primitive cell,
2 – the same as 0 followed by 1,
3 – the same as 2 plus relationships between solutions.
The default value of _SortSolutionsByQualityVsVolume is 0.

Besides the _NumberOfReflections, three other of the listed parameters have a large impact on the execution time. These are:

```
_MinMaxVolumeOfPrimitiveCell
_ExtentOfTheSearch
_FractionOfSupportingReflections
```

The last one influences only the time of testing individual volumes, but not the calculation of peri-odogram. The other two affect both phases. For high efficiency, one needs narrow bounds on the volume of the primitive cell and low values of the other two parameters.

Output file: A run of Ind_X on filename.idx will produce a file filename_idx.res. E.g., Ind_X example.idx gives example_idx.res. The output file contains a header with parameters of a given run and a number of proposed solutions.
• For each solution, one gets a matrix, say M, of basis vectors of the direct lattice (as matrix rows). This matrix is inverse to the 'orientation' matrix UB (i.e, $M = (UB)^{-1}$), where U and B are the conventional matrices of [W.R.Busing and H.A.Levy, Acta Cryst. **22**, 457–464 (1967)], and $M\times$ reciprocal lattice vector $\approx$ Miller indices of the reflection.
• Then, for each solution, there is a table of Miller indices corresponding to particular reflections. The 'Error' of a given reflection is represented by $|\,\mathbf{m} - \mathtt{NINT}(\mathbf{m})\,|$, where $\mathbf{m}$ is the triplet of real estimates of Miller indices.
• The 'Quality' of the solution equals to the ratio $(w_H N_H + w_h N_h)/(N(w_H + w_h))$, where N represents _NumberOfReflections.
• Finally, there are the conventional parameters a, b, c, α, β, γ of the primitive cell, and the volume of the primitive cell.

The solutions are sorted according to _SortSolutionsByQualityVsVolume. If this parameter equals 3, the output file contains information about relationships between particular solutions. The relationship between two solutions a and b with M_a and M_b (the matrices of basis vectors of their direct lattices) satisfying $|\det(M_a)| \geq |\det(M_b)|$ is represented by the matrix T such that $M_a = T\,M_b$. Miller indices of the solution b can be obtained by multiplying T and the column of indices of the solution a.