Function: IndX_Laue 0.1 is a prototype of a program for *ab initio* indexing of Laue diffraction pattern given in the form of normalized scattering vectors corresponding to detected Laue spots.

Operating system: MS Windows

Language: Fortran 90

Distribution: Free for academic use.

Method: A text on this subject is under preparation.

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

Input file: To learn the structure of the input file examine example.lpx. 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 321 reflections, one will have

```
_NumberOfReflections
       321
```

Then, the file must contain the keyword `_Reflections` and a list of reflections – normalized scattering vectors (corresponding to detected Laue spots) specified by their Cartesian coordinates

```
_Reflections
    0.82671760  0.41885773 -0.37562777
    0.11752733  0.91849288 -0.37756875
         ...        ...        ...
```

The list of optional keywords includes:

	Type	Range	Default
`_VolumeOfPrimitiveCell`	F		1000
`_MaxAllowedMillerIndex`	I	$[4, 30]$	12
`_AngularDeviationCriterion`	F	$[0.1, 3.0]$	1.0
`_WeightsForSortingBases`	F F	> 0.0	0.3 0.7
`_ExtentOfTheSearch`	I	$\{0, 1, 2, \ldots, 9\}$	0
`_MaxNumberOfSavedBases`	I	$[1, 128]$	16

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 keyword `_VolumeOfPrimitiveCell` must be followed by a line with the known or assumed volume of the primitive cell. For instance, assuming that the length is given in Å, the specification

```
_VolumeOfPrimitiveCell
     777.7
```

means that the volume of the primitive cell is assumed to be 777.7Å^3. The default volume is 1000Å^3.

• 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
     18
```

means that the absolute values of Miller indices will not exceed 18. The default value is 12.

• The keyword `_AngularDeviationCriterion` must be followed by a line with a single real number in the range [0.1, 3.0] specifying the allowed angular deviations of vectors obtained from ascribed Miller indices from experimental scattering vectors. For instance,

```
_AngularDeviationCriterion
     0.6
```

means that the allowed deviations cannot exceed 0.6°. Reflections with such deviations are marked in output files by `H-` or `-h`. Those with deviations not exceeding half of the specified value (0.3° in the above example) are marked by `H-`. The default value of `_AngularDeviationCriterion` is 1.0°.

• 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 `_ExtentOfTheSearch` must be followed by a line with an integer in the range from 0 to 9 specifying the extent of the search for the solution. E.g., one may have

```
_ExtentOfTheSearch
     3
```

By setting `_ExtentOfTheSearch` one chooses the method of search for the solution; see Tab. 1. The default value of `_ExtentOfTheSearch` is 0.

$M_{7,1}$	$M_{7,3}$	$M_{7,8}$	$M_{7,16}$	$M_{6b,1}$	$M_{6c,1}$	$M_{6c,3}$	$M_{6c,8}$	$M_{4,3}$	$M_{4,1}$
0	1	2	3	4	5	6	7	8	9

Table 1: The symbol $M_{k,I}$ means that the indexing was performed using k-tuplets of scattering vectors and superlattices of index I. $6b$ and $6c$ are two different types of sextuplets.

• 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.

Output file: A run of `IndX_Laue` on `filename.ldx` will produce a file `filename_ldx.res`. E.g., `IndX_Laue example.ldx` gives `example_ldx.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 $\widetilde{\propto}$ 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.

• With N representing `_NumberOfReflections`, the '`Quality`' of the solution equals to the ratio $(w_H N_H + w_h N_h)/(N(w_H + w_h))$ times a factor accounting for large disparities between fractions of odd and even indices.

• 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 their quality.