Function: KiKoCh2 is a program for crystal orientation determination based on indexing diffraction data given in the form of normalized scattering vectors. The data can be obtained from EBSD patterns, Kikuchi patterns, Laue patterns, Kossel patterns et cetera.

Files:
`KiKoCh2.pdf` – this file,
`KiKoCh2.exe` – 32-bit executable compiled under MS Windows,
`SEM_cub.kk2, TEM_hex_3.kk2, TEM_hex_4.kk2, SEM_ico.kk2` – example input files.

Distribution: Free for academic use.

Method: Described in *Acta Cryst.* **A76**, 719–734 (2020).

Execution: Run `KiKoCh2` and respond to the question about filename, or run `KiKoCh2 filename.kk2`. The filename must **not** contain spaces; otherwise, use `KiKoCh2 "filename with spaces.kk2"`. The extension `.kk2` is mandatory.

Input file: To learn the structure of an input file, examine one of the example input files. An input file contains keywords followed by appropriate data. The optional keywords are listed in Table below. (The type `I` denotes integers and `F` denotes floats.)

		Type	Range	Default
`_NumberOfBasisVectors`	n	`I`	$[3, 6]$	3
`_LatticeBasis`	$n \times 3$ matrix of	`F`		Identity matrix
`_NumberOfFamiliesOfReflectingPlanes`		`I`	$[1, 128]$	4
`_FamiliesOfReflectingPlanes`	list of n-tuples	`I`		(see below)
`_NumberOfSymmetryOperations`		`I`	$\geq 1,\ \leq 60$	24
`_SymmetryOperations`	list of quadruplets	`F`		point group O
`_IndexingStrategy`		`I`	$\{1, 2, 3, 4\}$	2
`_ParametersOfStrategy`	(in degrees)	`F F`	$[0.1°, 10.0°]$	1.0 2.0
`_NumberOfPatterns`		`I`	$[1, $`HUGE(I)`$]$	`HUGE(I)`

If present, the specification of the parameter `_NumberOfBasisVectors` must precede the keyword `_LatticeBasis`.
If present, the specification of the parameter `_NumberOfFamiliesOfReflectingPlanes` must precede `_FamiliesOfReflectingPlanes`.
If present, the specification of `_NumberOfSymmetryOperations` must precede the keyword `_SymmetryOperations`.

• The keyword `_NumberOfBasisVectors` must be followed by a line with an integer indicating the number of vectors determining the (quasi)lattice. For instance, one may have

```
_NumberOfBasisVectors
     4
```

This number cannot be smaller than 3 and it cannot exceed 6. If _NumberOfBasisVectors is used, the next keyword should be _LatticeBasis.

• The keyword _LatticeBasis must be followed by $n =$ _NumberOfBasisVectors lines with vectors $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}$ determining the direct (quasi)lattice. Each vector is represented by its three components in the Cartesian system $\mathbf{e}_i^c$ $(i = 1, 2, 3)$ attached to the crystal, i.e., the matrix M below _LatticeBasis has the entries $M_{ij} = \mathbf{a}_i \cdot \mathbf{e}_j^c$ $(i, j = 1, 2, 3)$. For instance, for hexagonal lattice of Zn (with lattice parameters in Å and _NumberOfBasisVectors=3) one may have

```
_LatticeBasis
      2.6649    0.0000    0.0000
     -1.3325    2.3079    0.0000
      0.0000    0.0000    4.9468
```

This means that the vectors are

$$\begin{aligned} \mathbf{a} &= \mathbf{a}_1 = \quad 2.6649\,\mathbf{e}_1^c + 0.0000\,\mathbf{e}_2^c + 0.0000\,\mathbf{e}_3^c\ , \\ \mathbf{b} &= \mathbf{a}_2 = -1.3325\,\mathbf{e}_1^c + 2.3079\,\mathbf{e}_2^c + 0.0000\,\mathbf{e}_3^c\ , \\ \mathbf{c} &= \mathbf{a}_3 = \quad 0.0000\,\mathbf{e}_1^c + 0.0000\,\mathbf{e}_2^c + 4.9468\,\mathbf{e}_3^c\ . \end{aligned}$$

Alternatively, in this case, one can use _NumberOfBasisVectors=4 vectors

```
_LatticeBasis
      2.6649    0.0000    0.0000
     -1.3325    2.3079    0.0000
     -1.3325   -2.3079    0.0000
      0.0000    0.0000    4.9468
```

The default _LatticeBasis is the identity matrix (cubic lattice).

• The keyword _NumberOfFamiliesOfReflectingPlanes must be followed by a line with an integer indicating the number of families of reflections expected to be detected in the diffraction pattern. For instance, one may have

```
_NumberOfFamiliesOfReflectingPlanes
     6
```

This number cannot be smaller than 1 and it cannot exceed 128.
If the keyword _NumberOfFamiliesOfReflectingPlanes is used, the next keyword should be _FamiliesOfReflectingPlanes.

• The keyword _FamiliesOfReflectingPlanes must be followed by lines with indices of families of reflecting planes (i.e., indices of high intensity peaks expected to be detected in the diffraction pattern). For a given family, the number of indices (i.e., the number of columns in the table) must be _NumberOfBasisVectors. For instance, with _NumberOfBasisVectors = 3, one may have

```
_FamiliesOfReflectingPlanes
      0    1    0
      0    0    2
      0    1    1
      0    1    2
      1    1    0
      0    1    3
```

which means that the families are $\{0\,1\,0\}$, $\{0\,0\,2\}$, $\{0\,1\,1\}$, $\{0\,1\,2\}$, $\{1\,1\,0\}$ and $\{0\,1\,3\}$.
If the keyword `_FamiliesOfReflectingPlanes` is used in a given data file, it must be preceded by the keyword `_NumberOfFamiliesOfReflectingPlanes`.
The default value of `_NumberOfFamiliesOfReflectingPlanes` is 4, and the default families of reflecting planes are $\{1\,1\,1\}$, $\{0\,0\,2\}$, $\{0\,2\,2\}$ and $\{1\,1\,3\}$.

• The keyword `_NumberOfSymmetryOperations` must be followed by a line with the number of proper rotations in the Laue (point) group of the crystal. For instance,

```
_NumberOfSymmetryOperations
      12
```

means that the number of proper rotations in the Laue group is 12.
If the keyword `_NumberOfSymmetryOperations` is used in a given file, the next keyword should be `_SymmetryOperations`.

• The keyword `_SymmetryOperations` must be followed by lines with symmetry operations of the Laue group. The operations are specified by the coordinates of the rotation axes in the Cartesian system $\mathbf{e}_i^c$ $(i = 1, 2, 3)$ attached to the crystal and the rotation angles in degrees. For instance, one may have

```
_SymmetryOperations
      0.0000   0.0000   1.0000       0.000
      0.0000   0.0000   1.0000      60.000
      0.0000   0.0000   1.0000     120.000
      ......   ......   ......     .......
```

i.e., the first symmetry is the identity operation, the second and third are rotations about $\mathbf{e}_3^c$ by the angles of 60° and 120°, respectively. If the keyword `_SymmetryOperations` is used, it must be preceded by the keyword `_NumberOfSymmetryOperations`.
The default value of `_NumberOfSymmetryOperations` is 24, and the default symmetry operations are those from the chiral octahedral point group O (432).

• The keyword `_IndexingStrategy` must be followed by one of the integers 1, 2, 3 or 4. The integer indicates the strategy to be used in computation. The numbers 1, 2, 3 and 4 correspond to the strategies A, B, C and D, respectively. For instance,

```
_IndexingStrategy
       2
```

means that the strategy B will be used. The default value of `_IndexingStrategy` is 2.

• The keyword `_ParametersOfStrategy` must be followed by a line with two positive real numbers specifying tolerances p_1 and p_2 used in indexing routines. For instance, if the data are

```
_ParametersOfStrategy
      2.0   1.1
```

the program will run with $p_1 = 2.0^\circ$ and $p_2 = 1.1^\circ$. The range of each of these tolerances is $[0.1^\circ, 10.0^\circ]$. The default values are $p_1 = 1.0^\circ$ and $p_2 = 2.0^\circ$.

• The keyword `_NumberOfPatterns` must be followed by a line with an integer specifying the number of patterns to be processed. For instance, with

```
_NumberOfPatterns
       100000
```

there should be at least 100000 data sets (patterns) in the section `_PatternData`; if there are more sets, only the first 100000 will be processed. The minimal value of `_NumberOfPatterns` is 1. The largest allowed (and default) value of `_NumberOfPatterns` is `HUGE(I)` (= 2147483647).

• Comments ignored by the program are allowed in the header of the input file before the keyword `_PatternData`. The lines with comments must begin with the character #.

• The **last** of the keywords must be `_PatternData`. It is mandatory, and it is followed by properly formatted data for individual diffraction patterns. For each pattern, there are
– a line with arbitrary content; it must be present but the content is not read,
– a line with the number of scattering vectors, say `N`,
– `N` lines, each with three components of nonzero scattering vectors specified by their Cartesian coordinates in sample reference frame $\mathbf{e}_i^s$ $(i = 1, 2, 3)$.
The number of scattering vectors `N` must be in the range $[2, 32]$. (The upper limit can be changed in the source code. It is specified there by the parameter `max_numOfScattVects`.)
The beginning of the data block may look like this

```
_PatternData
  Pattern no 1
   5
      0.5122664   0.5300164  -0.6757705
      0.8116305   0.5572611  -0.1752597
      0.8408079  -0.2067043  -0.5003153
     -0.5705720   0.7394485  -0.3573004
```

```
   -0.5049917   0.8383213  -0.2054283
Pattern no 2
 7
    0.5444633   0.8370910  -0.0532769
    0.2874883  -0.9149224  -0.2833151
    .........   .........   .........
```

Output file: A run of `KiKoCh2` on `filename.kk2` will produce a file `filename_kk2.res`. E.g., `KiKoCh2 example.kk2` gives `example_kk2.res`. After a header, the file contains results in the form of `_NumberOfPatterns` rows and seven columns. Each row corresponds to one data set (pattern).

```
=========================================================
---------------------------------------------------------

KiKoCh2 : Solutions for my_input_file.kk2

---------------------------------------------------------
        no      ph1_1     Phi   phi_2  used/all     fit
---------------------------------------------------------
         1      15.71   21.33  221.43    11  13   1.720
         2     111.21   32.36  253.64     9  14   1.564
         3      46.21   17.61  338.09     8   9   1.884
       ...     ......  ......  ......   ... ...   .....
```

The data in the columns are:
column 1 (`no`) – pattern number,
columns 2–4 (`ph1_1 Phi phi_2`) – Euler angles $\varphi_1, \phi, \varphi_2$ (in degrees) in Bunge's convention,
column 5 (`used`) – number of scattering vectors used in indexing,
column 6 (`all`) – number of scattering vectors provided in data file,
column 7 (`fit`) – approximate root mean square of angular deviations between used scattering vectors and the directions of corresponding reciprocal lattice vectors (in degrees).
The special orthogonal matrix $O = O(\varphi_1, \phi, \varphi_2)$ determined by the resulting Euler angles φ_1, ϕ and φ_2 relates the Cartesian reference frames $\mathbf{e}_i^s$ and $\mathbf{e}_i^c$ via $\mathbf{e}_i^c \approx \sum_j O_{ij} \mathbf{e}_j^s$. If `_NumberOfBasisVectors`=3, the indices $h\,k\,l = h_1\,h_2\,h_3$ of the reflection $\mathbf{s} = \sum_i s_i \mathbf{e}_i^s$ are $h_i \;\widetilde{\propto}\; \sum_{j,k} M_{ij}\, O_{jk}\, s_k$.
If there is no solution, the values of Euler angles are -1.00, the number of scattering vectors used in indexing is 0, and `fit` is set to 999.999.

```
        no      ph1_1     Phi   phi_2  used/all     fit
---------------------------------------------------------
       ...     ......  ......  ......   ... ...   .....
      3741      -1.00   -1.00   -1.00     0   4 999.999
       ...     ......  ......  ......   ... ...   .....
```