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Ind_X: program for indexing single-crystal diffraction patterns

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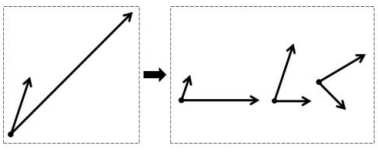
Indexing is an essential step in analysis of diffraction patterns. Diffraction of monochromatic radiation by a single crystal provides approximate positions of some nodes of the reciprocal lattice of the crystal, and the indexing problem lies in determining a lattice matching these positions. *Ind_X* is a program for indexing diffraction data given in the form of several approximate reciprocal lattice nodes. The applied method relies on testing potential volumes of the primitive cell of the reciprocal lattice. A subset of reciprocal lattice vectors supporting a given test volume is used to obtain tentative lattice bases. These are bases of low-index superlattices of lattices based on triplets of supporting vectors. The *Ind_X* solution of the indexing problem consists of a list of best bases. The method turns out to be quite robust to data inaccuracies and spurious reflections. The program is relatively versatile, easily operated and freely accessible.

1. Introduction

The process of ascribing Miller indices to reflections on diffraction patterns is referred to as indexing. Indexing appears in most diffraction-based crystallographic studies. In particular, it is an important element of structure determination by single-crystal diffraction of monochromatic X-rays. In this case, recorded data can be converted to vectors approximating the crystal reciprocal lattice, and the indexing is reduced to determination of the true lattice from several approximate positions of lattice nodes.

It must be noted at the outset that indexing of accurate reciprocal lattice vectors is straightforward. Complications arise when the diffraction data are inaccurate. Consistent and reliable indexing of error-affected input or cases with multiple lattices contributing to a pattern can be difficult. Robustness of indexing procedures to both random errors in locations of diffraction peaks and gross errors (inaccurate instrument settings, spurious reflections) is crucial for correctness of results.

Most indexing programs are just intrinsic parts of structure-determination packages (*e.g.* Pflugrath, 1999; Otwinowski & Minor, 2001; Leslie *et al.*, 2002; Kabsch, 2010), but also a number of standalone indexing tools have been reported (*e.g.* Klein, 1975; Duisenberg, 1992; Pilz *et al.*, 2002; Sauter *et al.*, 2004). *Ind_X* is a program for indexing diffraction data given in the form of reciprocal lattice nodes. It was written to extend the capabilities of a software package for analysis of Kossel diffraction patterns (Morawiec, 2016). The intended application was lattice parameter determination, and it concerned relatively simple crystal structures. However, additional tests on simulated diffraction data showed that the program is also applicable to more complicated indexing problems. *Ind_X* can



be compared to *DirAx* (Duisenberg, 1992), which is considered to be most suitable for solving difficult cases. Our tests indicate that *Ind_X* has a similar effectiveness in this regard. For illustration, see the supporting information with solutions for the example data of Duisenberg (1992).

Each indexing program has specific built-in mechanisms for controlling the extent of search for solutions. In some cases, the choice of the control parameters and criteria is essential for getting the right result, and it is important to have diverse instruments for solving such patterns. *Ind_X* adds to the diversity of available indexing tools. Since the program is compact and easily operated, it can be conveniently used for solving small-cell problems. An important feature of *Ind_X* is the simplicity of the applied method.

2. Method

Numerous indexing schemes have been considered in the past (see *e.g.* Jacobson, 1976; Vriend & Rossmann, 1987; Kabsch, 1988; Kim, 1989; Higashi, 1990; Duisenberg, 1992; Steller *et al.*, 1997; Jacobson, 1997; Campbell, 1998; Powell, 1999; Gildea *et al.*, 2014). The procedure implemented in *Ind_X* relies on the volume of the primitive cell of the reciprocal lattice. The initial test volumes can be either automatically determined by the program or provided by the user.

The first approach (automatic determination) is based on period-detection methods. In the error-free case, the volume of the primitive cell would be a submultiple of volumes of parallelepipeds spanned by reciprocal lattice vectors, *i.e.* the latter volumes would be distributed periodically. In practice, the volumes of such parallelepipeds are affected by experimental errors, and the volume distributions show some periodicities but are not exactly periodic. The point is to find the period of the distribution obtained from experimental reciprocal lattice vectors. The volumes calculated by *Ind_X* from triplets of experimental vectors constitute a data series, and to get the period the program uses a periodogram – the primary tool for identification of periodicities in data series (Anderson, 1971). In the considered case, the periodogram can be seen as the frequency of occurrence of particular periods among volumes of parallelepipeds spanned by triplets of the experimental reciprocal lattice vectors. For accurate diffraction data, such periodograms have simple structures, and it is easy to determine the period. For many experimental data sets, however, periodograms tend to be noisy (Fig. 1). Therefore, *Ind_X* extracts a number of test volumes corresponding to the highest peaks of a given periodogram.

Alternatively, the test volumes can be indicated by the user based on visual inspection of a periodogram. If the periodogram is noisy, one may provide a list of (up to 350) properly distributed volumes. On the other hand, the list may contain a single volume if, after getting an indexing solution, one decides to check whether there are any twin-related solutions; the latter correspond to the same volume as the initial solution, so the check is done by running *Ind_X* for this particular test volume. The test volumes do not need to be accurate as the initial set of test volumes is extended by volumes in the vicinity of those in the initial set; this applies to both user-provided and automatically determined volumes.

For each test volume, the program selects a subset of reciprocal lattice vectors supporting it. Roughly, a vector supports a test volume if it is comprised in numerous triplets spanning parallelepipeds with volumes close to integer multiples of the test volume. The program estimates the quality of support by an individual vector by checking all triplets in which the vector is comprised. The larger the number of parallelepipeds with

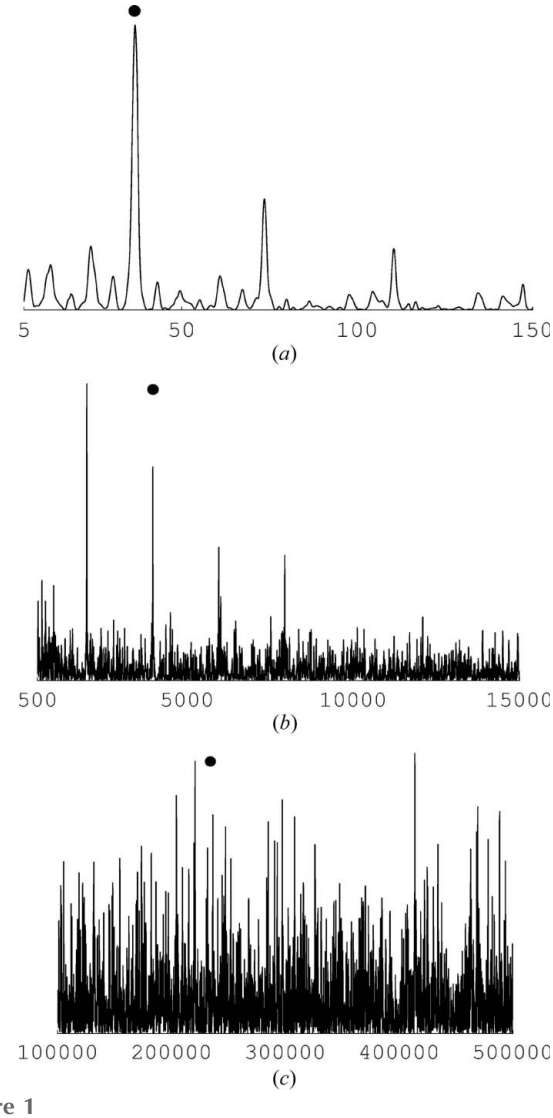


Figure 1
Example Lomb–Scargle periodograms in arbitrary units *versus* volume in direct space (Å^3). Plots are shown in ranges which one may select on the basis of the type of crystal or the density of reflections. Discs mark volumes of parallelepipeds spanned on primitive bases of best lattices. (*a*) Periodogram obtained from 16 vectors corresponding to conics in a Kossel diffraction pattern of the martensite phase of Cu–Al–Be alloy (Bouscaud *et al.*, 2014). The smallest primitive cell volume allowing for indexing of the pattern was about 3.7×10^1 Å^3. (*b*) Periodogram for 30 reflections from a simulated diffraction data set of a crystal with a cell of medium size, 4.0×10^3 Å^3. (*c*) Periodogram based on 26 reflections from 'Example 2' of Duisenberg (1992), representing a small protein with a cell volume of about 2.3×10^5 Å^3.

volumes close to integer multiples of the test volume, the larger the support.[1] The vectors are then ranked, and the best vectors constitute the needed subset. The reasons for using the subset of supporting vectors are twofold: first, the subsequent confinement to this subset eliminates potential spurious reflections, and second, it speeds up the program.

The supporting vectors are used to construct tentative solutions. Briefly, the tentative bases of the reciprocal lattice are bases of low-index superlattices of the lattices based on triplets of the supporting vectors. The scheme is illustrated two dimensionally in Fig. 2. A triplet of legitimate vectors [like the vectors in Fig. 2(*a*)] determines a certain lattice (Fig. 2*b*). Trivial but crucial for what follows is the observation that this lattice is a sublattice of the actual reciprocal lattice of the crystal [Fig. 2(*b*) shows a sublattice of the lattices shown in Fig. 2(*c*)]. Thus the indexing problem is reduced to checking all bases of small-index superlattices of the lattice based on the triplet. [This corresponds to checking the bases shown in Fig. 2(*d*).] For details on generation of superlattices in the three-dimensional space see, for example, Santoro & Mighell (1973) and Billiet & Coz (1980). Since the number of superlattices grows fast with the index,[2] the program checks the bases of superlattices up to index 3 in the quickest case, up to 7 by default and up to 16 in the most extensive calculations. The construction of the solutions also includes two standard steps: fitting integer combinations of basis vectors to the supporting vectors (Kim, 1989) and Buerger reduction of the basis (Buerger, 1957, 1960). Having a tentative basis, indexing of all experimental reflections is attempted. The result of the attempt is used to quantify the quality of the basis. The bases of highest quality are saved. The number of saved bases is controlled by the user (but it cannot exceed 128). These steps are repeated for all tentative bases constructed from a given triplet of supporting vectors, for all triplets of vectors supporting a given test volume and for all test volumes.

As for the important parameter representing the quality of a basis, a number of different quantities have been tested to find a balance between effectiveness, simplicity and flexibility. The implemented approach is based on a user-controlled limit on the allowed deviation of Miller indices from integers. With the number of reflections within this limit denoted by N_h and the number of reflections within half of the limit denoted by N_H, the quality of the basis is proportional to $w_H N_H + w_h N_h$, where w_H and w_h are user-controlled weights.

Ind_X can only process data sets containing a relatively small number of reflections N because the number of reflection triplets grows with N as N^3, and this has an impact on the execution time. Typically, N is expected to be about 20–50. With a small number of reflections and suitably chosen *Ind_X* parameters (see below), the execution time can be a fraction of a second. However, one must be aware that speed comes at a price of quality. For higher reliability of results, one can perform an extended search, and this can be a lengthy process.

3. Software and hardware environment

Ind_X is written in Fortran 90. It can be run from a command prompt in a console window on personal computers under

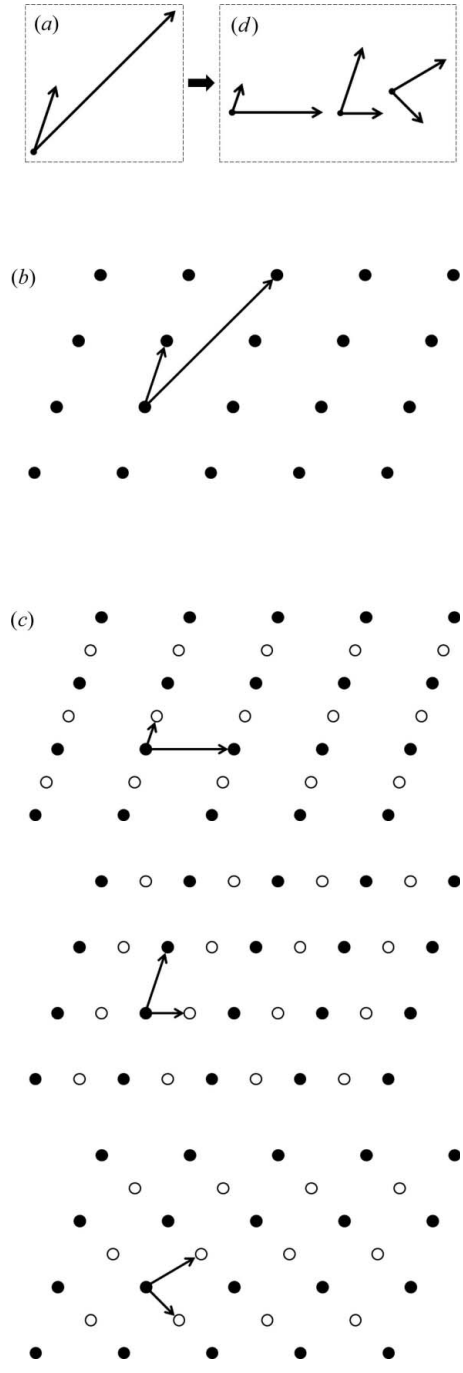


Figure 2
Schematic two-dimensional illustration of the construction of tentative bases from the two 'experimental' reciprocal lattice vectors drawn in (*a*). The lattice based on the two vectors is represented by discs in (*b*). Its three superlattices (discs + circles) of index 2 are shown in (*c*). The three bases of the superlattices are used as tentative bases (*d*).

[1] In other words, if the test volume corresponds to a peak in the periodogram, the support is large if the vector contributed numerous times (*i.e.* as a member of numerous triplets) to the peak.
[2] For example, for the indices 3, 5, 7, 10 and 16, the number of superlattices is 13, 31, 57, 217 and 651, respectively (*cf.* Santoro & Mighell, 1973).

Microsoft Windows operating systems. The program uses a single input file with keywords followed by appropriate data. The file must contain a set of reflections specified by Cartesian coordinates of reciprocal lattice vectors. There are also a number of optional input parameters, like the above-mentioned limit on the allowed deviation of a Miller index from an integer or the largest allowed absolute value of Miller indices. Besides the number of reflections, three optional parameters have an impact on the execution time. These are (1) limits on the allowed volume of the primitive cell, (2) an upper limit on the number of supporting reflections and (3) a single entity controlling (through a number of secondary parameters) the extent of the search for the solution. In particular, the latter entity determines the density of arguments of the periodogram, the number of automatically detected test volumes and the upper limit on the index of inspected superlattices.

A typical output file contains a list of proposed solutions. The choice of the ultimate solution from the list is left to the user. For each solution, one gets a matrix of basis vectors of the direct lattice.[3] Then, there is a table of Miller indices corresponding to particular reflections, the parameters a, b, c, α, β and γ, and the volume of the primitive cell. The program delivers the Buerger-reduced cell, and additional processing is needed to obtain the lattice symmetry. The task can be performed using *LEPAGE* (Spek, 1988) or other procedures of this kind (see *e.g.* Clegg, 1981; Le Page, 1982; Zimmermann & Burzlaff, 1985; Higgins *et al.*, 1990; Macíček & Yordanov, 1992).

4. Availability

A 0.22 MB compressed file with the executable `Ind_X.exe` for Windows can be downloaded from http://imim.pl/personal/adam.morawiec/. Program documentation is limited to PDF-formatted instructions. Alternatively, one can download a 0.52 MB package which, besides `Ind_X.exe`, contains a .NET-based graphical user interface written by M. F. Morawiec. The interface facilitates changes of *Ind_X* parameters and analysis of periodograms.

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[3] This matrix is inverse to the **UB** matrix of Busing & Levy (1967); the product of the saved $(\mathbf{UB})^{-1}$ with an experimental reciprocal lattice vector gives approximate Miller indices of the corresponding reflection.

Supplementary material

(to '*Ind_X*: program for indexing single crystal diffraction patterns' by A. Morawiec)

Tables below show high quality solutions (parts of output files) obtained by running *Ind_X* for data of Duisenberg (1992). In response to a recommendation by an anonymous reviewer, also results for unpublished "examples 6 and 7" are listed. In all cases, the limit on the allowed deviation of Miller indices from integers was the *Ind_X* default of 0.12; reflections within this limit are denoted by `-h` and reflections within half of the limit are denoted by `H-`. The unit of length is Ångström, and angles are in degrees.

Example 1:

```
 Solution nr   2 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -0.41624538    0.04542523    5.05672819
            -2.24425594   -7.88469324   -0.11196100
           -11.93485938    1.08178703   -0.99071084

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   2   0  -8 |   2.01   0.00  -8.03  |  0.032
  2  H- |   2  -5  -7 |   2.00  -5.00  -6.96  |  0.037
  3     |             |   1.97  -0.01  -9.20  |  0.205
  4
  5  H- |   1  -1  -7 |   0.99  -1.00  -6.94  |  0.058
  6
  7  H- |   1   0  -7 |   1.00   0.00  -7.03  |  0.032
  8  H- |   1  -2  -7 |   1.00  -2.00  -7.00  |  0.004
  9  -h |   2  -3   3 |   1.93  -3.00   2.93  |  0.093
 10  H- |   3  -4   0 |   3.01  -4.00   0.04  |  0.039
 11  H- |   1  -4   1 |   1.01  -4.00   0.95  |  0.055
 12  H- |   1  -4   0 |   0.99  -4.00   0.04  |  0.044
 13  -h |   1  -4   0 |   1.01  -4.00  -0.07  |  0.074
 14  H- |   2  -1   4 |   2.01  -1.00   4.02  |  0.026
 15     |             |   1.93   0.00   4.22  |  0.232
 16  H- |   2  -3  -2 |   2.01  -3.00  -1.98  |  0.025
 17  H- |   3   1   6 |   3.02   1.00   5.99  |  0.021
 18  -h |   2   0   8 |   2.01   0.01   8.07  |  0.073
 19
 20  H- |   1   1   6 |   1.00   1.00   6.00  |  0.004
 21  H- |   1   4  -1 |   0.98   4.01  -0.99  |  0.026
 22     |             |   1.97   1.99   2.22  |  0.226
 23  H- |   2   1   1 |   1.99   0.99   0.94  |  0.061
 24  H- |   3   2   1 |   3.00   2.00   0.99  |  0.011
 25     |             |   3.04   1.99  -2.16  |  0.166
-------------------------------------------------------
  18h and  15H vectors out of  25.    Quality : 0.684

 Primitive cell :
                         5.074    8.199   12.025
                        79.26    89.99    89.99

 Volume of the cell  :      491.47
```

Example 2:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            22.39827411   23.67373447   19.86433441
           -55.72013365   53.74568735    2.85453230
            27.36701652   32.99645419  -66.67913680

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
 1  -h |   0   4   7 |  -0.02   3.92   6.89  |  0.134
 2  H- |   3  15  11 |   3.01  15.01  10.99  |  0.017
 3  H- |   4  24  14 |   4.01  24.03  14.01  |  0.031
 4  -h |   1   6   7 |   0.99   5.94   6.91  |  0.105
 5  H- |   6  15   0 |   6.00  14.95  -0.04  |  0.059
 6  -h |   5  22  10 |   4.99  22.05  10.09  |  0.100
 7  H- |   4  27  15 |   4.01  27.00  14.97  |  0.037
 8  -h |   7  26   5 |   7.00  26.05   5.07  |  0.090
 9  -h |   9  27  -6 |   9.00  26.91  -6.10  |  0.131
10  -h |   6  29  10 |   6.01  29.11  10.03  |  0.116
11  -h |   5  24  11 |   4.99  24.03  11.08  |  0.090
12  -h |   1  26  21 |   0.98  25.90  20.92  |  0.126
13  -h |   6  13  -3 |   6.01  12.98  -3.08  |  0.079
14  H- |   4  15   8 |   4.00  15.02   8.03  |  0.030
15  -h |   3   5  -2 |   3.00   4.98  -2.06  |  0.066
16  H- |   4   7  -3 |   4.00   6.99  -3.05  |  0.054
17  H- |   4   8  -1 |   4.00   8.00  -1.02  |  0.020
18  H- |   7  23   3 |   7.00  22.98   3.03  |  0.040
19  H- |   6  10 -11 |   5.98   9.96 -11.02  |  0.051
20  H- |   5  13   2 |   5.00  12.98   1.99  |  0.021
21  H- |   6  20   5 |   6.00  20.00   5.05  |  0.049
22  -h |   2  26  19 |   2.00  25.93  18.93  |  0.101
23  H- |   8  28   1 |   8.01  28.01   1.02  |  0.023
24  -h |   8  30   2 |   8.00  30.09   2.08  |  0.118
25  H- |   3  13   9 |   3.00  13.00   9.01  |  0.008
26  H- |   7  16  -5 |   7.00  15.95  -5.05  |  0.074
-------------------------------------------------------
  26h and  14H vectors out of  26.    Quality : 0.862

 Primitive cell :
                         38.167   77.469   79.271
                         89.46    88.68    88.43

 Volume of the cell  :   234225.58
```

Example 3, solution *a*:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -0.08757438    2.89242892   -3.33163710
            18.02074562   -1.42129210    1.17612284
            -3.89689517  -16.76216719  -11.52746836

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   1   3  -7 |   1.00   3.02  -6.99  |  0.023
  2  H- |   1  -3  -4 |   1.00  -2.99  -4.00  |  0.008
  3  H- |   0   5  -5 |   0.00   5.00  -5.00  |  0.004
  4  H- |   1  -3  -8 |   1.00  -3.00  -8.00  |  0.007
  5  H- |   0   0  -8 |   0.00   0.00  -8.00  |  0.003
  6  H- |   0  -5  -7 |   0.00  -5.00  -7.00  |  0.003
  7  H- |   0  -5  -3 |   0.00  -5.00  -3.00  |  0.005
  8  H- |   0   0 -12 |   0.00   0.00 -11.99  |  0.006
  9  H- |  -1   4  -6 |  -1.00   4.02  -6.00  |  0.016
 10  H- |  -1  -6  -8 |  -1.00  -5.99  -8.00  |  0.012
 11  H- |  -1  -7  -6 |  -1.00  -7.01  -6.00  |  0.012
 12  H- |   0   0 -12 |   0.00  -0.01 -12.01  |  0.016
 13  H- |   0   5 -13 |   0.00   5.00 -13.00  |  0.007
 14  H- |   1   2 -13 |   1.00   2.00 -13.00  |  0.003
 15  H- |   1   0 -13 |   1.00  -0.04 -13.01  |  0.036
 16  H- |   1  -3 -12 |   1.00  -3.00 -11.99  |  0.005
 17  H- |   1   1 -11 |   1.00   0.98 -11.01  |  0.019
 18  H- |  -1   3  -8 |  -1.00   3.00  -8.00  |  0.007
 19  H- |  -1   4 -10 |  -1.00   4.01  -9.99  |  0.014
 20  H- |   0  10 -10 |   0.00  10.00 -10.00  |  0.003
 21  H- |   1  -7  -9 |   1.00  -6.98  -9.00  |  0.023
 22  H- |   1   3 -11 |   1.00   3.02 -11.00  |  0.025
 23  H- |   1  -3  -8 |   1.00  -3.00  -8.00  |  0.003
 24  H- |   1   2  -9 |   1.00   2.01  -9.00  |  0.006
 25  H- |   1   1  -7 |   1.00   0.98  -7.00  |  0.016
-------------------------------------------------------
  25h and  25H vectors out of  25.    Quality : 1.000

 Primitive cell :
                          4.413   18.115   20.713
                         99.20    96.11    96.90

 Volume of the cell  :     1609.27
```

Example 4:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            1.20056709    1.71918935  -10.94962184
           -0.92071771  -22.25549176   -3.59537022
           97.65751543   -5.77590232    9.77179118

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   0  -3 -21 |   0.00  -3.02 -21.06  |  0.059
  2  H- |   0  -3 -24 |   0.00  -3.01 -23.99  |  0.011
  3     |             |   0.00  -3.04 -22.14  |  0.143
  4  H- |   0  -3 -23 |   0.00  -3.00 -22.98  |  0.023
  5  H- |   0  -5 -16 |   0.00  -5.00 -15.99  |  0.009
  6  H- |   0  -4 -26 |   0.00  -4.00 -25.95  |  0.050
  7  H- |   0  -1 -29 |   0.00  -1.01 -28.97  |  0.031
  8  -h |   0  -1 -31 |  -0.01  -0.89 -31.03  |  0.112
  9  H- |   0   0 -22 |   0.00  -0.01 -21.97  |  0.035
 10  H- |  -1  -4  18 |  -1.00  -3.99  17.98  |  0.022
 11  H- |  -1  -4  17 |  -1.00  -3.99  16.99  |  0.014
 12  H- |  -1  -5  11 |  -1.00  -4.99  11.00  |  0.007
 13  H- |  -1  -5  10 |  -1.00  -5.01  10.02  |  0.025
 14  H- |  -2   1 -19 |  -2.00   1.00 -18.97  |  0.025
 15  H- |  -2   0 -21 |  -2.00   0.00 -20.99  |  0.010
 16  H- |  -2   1 -23 |  -2.00   1.00 -22.96  |  0.037
 17  H- |  -2   0 -23 |  -2.00   0.00 -22.98  |  0.020
 18  H- |  -1  -3  27 |  -1.00  -2.99  27.00  |  0.015
 19  H- |   2  -2  19 |   2.00  -2.00  19.00  |  0.004
 20  H- |   2  -3  16 |   2.00  -3.00  16.01  |  0.011
 21  H- |   2  -4  11 |   2.00  -4.00  11.05  |  0.047
 22  H- |   2  -3  17 |   2.00  -3.00  17.01  |  0.013
 23  H- |   2  -4   9 |   2.00  -4.00   9.01  |  0.010
 24  H- |   2  -5   0 |   2.00  -5.01   0.01  |  0.014
 25  H- |   2  -4  15 |   2.00  -3.99  15.00  |  0.007
-------------------------------------------------------
  24h and  23H vectors out of  25.    Quality : 0.948

 Primitive cell :
                        11.149   22.563   98.315
                        89.91    89.98    90.00

 Volume of the cell  :    24730.50
```

The diffraction data of Example 3 were known to originate from an incommensurate structure. According to (Duisenberg 1992), a "supercell" fitting all reflections has the "volume $3942.00 = 49 \times 80.44$". The quite accurate *Ind_X* solution (a) shown above gives a smaller volume ($1609.27 \approx 20 \times 80.46$). If 100 is the upper limit on the cell volume, *Ind_X* gives the solution (b) with the volume of 80.43; see below. The relationship between the two solutions is $\mathbf{M}_a \approx \mathbf{T} \times \mathbf{M}_b$, where $\mathbf{M}_a$ and $\mathbf{M}_b$ are the matrices of direct lattice vectors (in rows) for each of the solutions, and

$$\mathbf{T} = \begin{bmatrix} 1 & -1 & 0 \\ -3 & -2 & 0 \\ 0 & 1 & 4 \end{bmatrix};$$

Miller indices of the solution (a) can be obtained by multiplying $\mathbf{T}$ and the column of indices of the solution (b). The smallest-volume solution accepting all reflections with the default *Ind_X* parameters is listed below as (c).

Example 3, solution *b*:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -3.63857749    1.44382309   -1.57287407
            -3.55149346   -1.44846389    1.75859322
            -0.08637420   -3.83006631   -3.31877056

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1
  2  H- |   1   0  -1 |   1.00   0.00  -1.00  |  0.001
  3  H- |  -1  -1  -1 |  -1.00  -1.00  -1.00  |  0.001
  4  H- |   1   0  -2 |   1.00   0.00  -2.00  |  0.001
  5  H- |   0   0  -2 |   0.00   0.00  -2.00  |  0.001
  6  H- |   1   1  -2 |   1.00   1.00  -2.00  |  0.001
  7  H- |   1   1  -1 |   1.00   1.00  -1.00  |  0.002
  8  H- |   0   0  -3 |   0.00   0.00  -3.00  |  0.002
  9
 10
 11  H- |   1   2  -2 |   1.00   2.00  -2.00  |  0.001
 12  H- |   0   0  -3 |   0.00   0.00  -3.00  |  0.003
 13  H- |  -1  -1  -3 |  -1.00  -1.00  -3.00  |  0.001
 14  H- |   0  -1  -3 |   0.00  -1.00  -3.00  |  0.000
 15
 16  H- |   1   0  -3 |   1.00   0.00  -3.00  |  0.001
 17
 18  H- |  -1   0  -2 |  -1.00   0.00  -2.00  |  0.001
 19
 20  H- |  -2  -2  -2 |  -2.00  -2.00  -2.00  |  0.001
 21
 22
 23  H- |   1   0  -2 |   1.00   0.00  -2.00  |  0.001
 24  H- |   0  -1  -2 |   0.00  -1.00  -2.00  |  0.000
 25
-------------------------------------------------------
  16h and  16H vectors out of  25.    Quality : 0.640

 Primitive cell :
                         4.219    4.219    5.069
                        89.95    89.99    63.06

 Volume of the cell  :       80.43
```

Example 3, solution *c*:

```
 Solution nr   9 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
             0.08764924   -2.89243836    3.33158017
            -7.09574696    3.84139431    3.45898860
            10.99137244   12.92062820    8.06968392

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |  -1   0   7 |  -1.00   0.05   6.94  |  0.076
  2  H- |  -1   2   2 |  -1.00   2.00   2.00  |  0.007
  3  H- |   0  -1   6 |   0.00  -1.00   6.00  |  0.003
  4  H- |  -1   3   5 |  -1.00   3.00   4.99  |  0.005
  5  H- |   0   2   6 |   0.00   1.99   6.01  |  0.010
  6  H- |   0   4   3 |   0.00   3.99   3.01  |  0.016
  7  H- |   0   3   0 |   0.00   2.99   0.01  |  0.010
  8  H- |   0   3   9 |   0.00   2.99   9.01  |  0.015
  9  H- |   1   0   6 |   1.00   0.02   5.97  |  0.037
 10  H- |   1   5   3 |   1.00   5.02   2.98  |  0.025
 11  H- |   1   5   1 |   1.00   4.98   1.02  |  0.032
 12  H- |   0   3   9 |   0.00   2.99   9.02  |  0.019
 13  H- |   0   1  12 |   0.00   0.99  12.01  |  0.013
 14  H- |  -1   2  11 |  -1.00   2.00  11.00  |  0.003
 15  -h |  -1   3  10 |  -1.00   2.92  10.09  |  0.121
 16  H- |  -1   4   8 |  -1.00   4.00   8.00  |  0.003
 17  H- |  -1   2   9 |  -1.00   1.96   9.04  |  0.057
 18  H- |   1   1   7 |   1.00   0.98   7.02  |  0.028
 19  H- |   1   1   9 |   1.00   1.02   8.97  |  0.036
 20  H- |   0  -2  12 |   0.00  -2.00  12.00  |  0.003
 21  H- |  -1   5   4 |  -1.00   5.04   3.96  |  0.058
 22  H- |  -1   1  10 |  -1.00   1.04   9.96  |  0.062
 23  H- |  -1   3   5 |  -1.00   3.00   5.00  |  0.004
 24  H- |  -1   1   8 |  -1.00   1.00   7.99  |  0.008
 25  H- |  -1   1   6 |  -1.00   0.97   6.04  |  0.049
-------------------------------------------------------
  25h and  24H vectors out of  25.    Quality : 0.988

 Primitive cell :
                         4.413    8.779   18.785
                        90.15    96.60    90.31

 Volume of the cell  :      722.90
```

Examples 6 and 7 are described at http://www.crystal.chem.uu.nl/distr/dirax/examples.html as "inaccurate data" and "not very accurate data", respectively. *DirAx* solutions to these examples are available at the same web page. The first solution given by *Ind_X* to example 6 is similar to that given by *DirAx*; in both cases, one reflection is not indexed. Example 7 is fully indexable (solution no 1). However, solutions 2 and 3 of *Ind_X* indicate that the data originate from a twinned crystal. Only solutions similar to 1 and 2 are listed at http://www.crystal.chem.uu.nl/distr/dirax/examples.html and, in consequence, the possibility of twinning is overlooked.

Example 6:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -0.22772791    0.41128973    3.87525272
            -0.28186242   -5.94601285    1.00932446
            16.69620088   -2.75388915    1.71750269

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   2   0  10 |   2.00   0.00  10.00  |  0.007
  2  H- |   2   2   9 |   2.00   2.00   9.01  |  0.011
  3  H- |   1  -1  13 |   1.00  -1.01  13.00  |  0.007
  4  H- |   0   2   6 |  -0.03   2.00   5.98  |  0.033
  5  H- |   0   3   4 |  -0.03   3.00   3.96  |  0.049
  6  H- |   0   1   9 |  -0.02   1.00   9.01  |  0.022
  7  H- |   1   1   5 |   0.99   1.00   4.98  |  0.021
  8  H- |   1   0   5 |   0.99   0.01   5.00  |  0.016
  9  H- |   2  -2  -2 |   2.02  -2.00  -2.02  |  0.028
 10
 11  H- |   1  -2   2 |   0.99  -2.00   2.01  |  0.012
 12  H- |   0  -2  -6 |  -0.02  -2.00  -6.00  |  0.022
 13  H- |   0  -1  -3 |  -0.02  -1.01  -2.99  |  0.026
 14  H- |   1  -1  -1 |   1.01  -1.00  -1.01  |  0.013
 15  H- |   0  -3   5 |  -0.01  -3.00   5.02  |  0.022
 16  H- |   0  -3  -4 |  -0.02  -3.00  -3.99  |  0.020
 17  H- |   2   1  -7 |   2.00   1.00  -7.00  |  0.005
 18  H- |   1   4  -1 |   0.98   4.00  -0.99  |  0.019
 19  H- |   2   3  -2 |   2.00   3.00  -1.99  |  0.013
 20  H- |   1   5   4 |   0.98   5.00   4.05  |  0.052
 21  -h |   1   4  -4 |   0.99   4.01  -4.12  |  0.120
 22  H- |   1   0  -8 |   0.99   0.00  -8.00  |  0.012
 23  -h |   1   2  -5 |   0.98   2.01  -5.12  |  0.117
 24  H- |   1   4  -7 |   0.98   4.02  -6.97  |  0.041
 25  H- |   0  -1  -6 |  -0.03  -1.01  -6.02  |  0.035
-------------------------------------------------------
  24h and  22H vectors out of  25.    Quality : 0.936

 Primitive cell :
                         3.904    6.038   17.009
                        82.50    88.51    86.28

 Volume of the cell  :      396.55
```

Example 7:

```
 Solution nr   1 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            1.84344954    3.25703922    8.82866263
           22.22374211    1.60108683   -5.22574341
           16.66747588  -35.84753215    9.80100707

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   4  10  24 |   4.01   9.99  23.98  |  0.024
  2  H- |   6  12  16 |   6.00  12.00  16.02  |  0.018
  3  H- |   4  12  22 |   4.01  11.99  21.97  |  0.034
  4  H- |   4   8  20 |   4.00   8.00  19.99  |  0.015
  5  H- |   6   7   1 |   6.00   7.02   1.04  |  0.049
  6  H- |   7  10   6 |   6.99  10.02   6.00  |  0.021
  7  H- |   5  15  15 |   5.00  14.99  14.98  |  0.017
  8  H- |   5  15  16 |   4.99  14.99  15.96  |  0.041
  9  H- |   4 -14 -16 |   4.00 -14.00 -16.03  |  0.033
 10  H- |   5 -11 -17 |   5.00 -11.00 -17.01  |  0.014
 11  H- |   5 -13 -21 |   5.00 -13.00 -21.02  |  0.023
 12  H- |   7   4 -14 |   7.00   4.00 -14.00  |  0.005
 13  H- |   6   2 -12 |   6.01   2.00 -11.97  |  0.029
 14  H- |   4 -13  -9 |   4.00 -13.00  -9.06  |  0.055
 15  H- |   5  -9 -14 |   5.00  -9.00 -13.96  |  0.041
 16  H- |   7  -4 -18 |   7.00  -4.01 -17.96  |  0.044
 17  H- |   2  -4  30 |   2.00  -4.00  30.02  |  0.020
 18  H- |   2  -5  29 |   2.00  -5.00  29.03  |  0.027
 19  H- |   2 -16   8 |   1.99 -16.01   8.00  |  0.010
 20  H- |   2 -16  10 |   1.99 -16.00   9.96  |  0.038
 21  H- |   1 -10  20 |   1.00  -9.99  19.99  |  0.013
 22  H- |   1 -12  16 |   1.00 -11.99  16.03  |  0.034
 23  H- |   2 -17  -5 |   2.01 -17.01  -5.04  |  0.039
 24  H- |   1 -13   8 |   1.00 -13.00   8.06  |  0.058
 25  H- |   1 -12  10 |   1.00 -11.99  10.01  |  0.012
-------------------------------------------------------
  25h and  25H vectors out of  25.    Quality : 1.000

 Primitive cell :
                         9.589   22.886   40.730
                        73.69    89.93    89.99

 Volume of the cell  :     8578.63
```

Example 7:

```
 Solution nr   2 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            -1.84244579   -3.25710729   -8.82838295
            -2.78455888  -18.72373301    7.51579641
            22.22271405    1.60042838   -5.22626771

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |  -4   7  10 |  -4.01   6.99   9.99  |  0.015
  2  H- |  -6   2  12 |  -5.99   2.01  12.00  |  0.010
  3  H- |  -4   5  12 |  -4.01   4.98  11.99  |  0.019
  4  H- |  -4   6   8 |  -4.00   5.99   8.00  |  0.012
  5  H- |  -6  -3   7 |  -6.00  -2.99   7.02  |  0.022
  6  H- |  -7  -2  10 |  -6.99  -2.01  10.02  |  0.024
  7  H- |  -5   0  15 |  -5.00  -0.01  14.99  |  0.011
  8
  9  H- |  -4  -1 -14 |  -4.00  -1.01 -13.99  |  0.015
 10  H- |  -5  -3 -11 |  -5.00  -3.00 -11.00  |  0.003
 11  H- |  -5  -4 -13 |  -5.00  -4.00 -13.00  |  0.006
 12  H- |  -7  -9   4 |  -7.00  -9.00   4.00  |  0.003
 13  H- |  -6  -7   2 |  -6.01  -6.99   2.00  |  0.014
 14  H- |  -4   2 -13 |  -4.00   1.98 -13.00  |  0.023
 15
 16  H- |  -7  -7  -4 |  -7.00  -6.97  -4.01  |  0.030
 17  H- |  -2  17  -4 |  -2.00  17.01  -4.00  |  0.013
 18  H- |  -2  17  -5 |  -2.00  17.02  -5.00  |  0.018
 19  H- |  -2  12 -16 |  -2.00  12.01 -16.01  |  0.012
 20  H- |  -2  13 -16 |  -1.99  12.99 -16.00  |  0.015
 21  H- |  -1  15 -10 |  -1.00  14.99  -9.99  |  0.012
 22  H- |  -1  14 -12 |  -1.00  14.01 -11.99  |  0.019
 23  H- |  -2   6 -17 |  -2.01   5.99 -17.01  |  0.015
 24
 25  H- |  -1  11 -12 |  -1.00  11.00 -11.99  |  0.009
-------------------------------------------------------
  22h and  22H vectors out of  25.    Quality : 0.880

 Primitive cell :
                          9.589   20.367   22.885
                        106.34    90.00    90.07

 Volume of the cell  :     4288.81
```

Example 7:

```
 Solution nr   3 out of  16.

  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
            1.84235217    3.25747591    8.82920015
            8.34452110  -17.93160379    4.89513606
           22.22639387    1.60217130   -5.22661136

        |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1  H- |   4  12  10 |   4.01  12.00   9.99  |  0.012
  2  H- |   6   8  12 |   6.00   8.01  12.00  |  0.014
  3  H- |   4  11  12 |   4.01  10.99  11.99  |  0.014
  4  H- |   4  10   8 |   4.00  10.00   8.00  |  0.006
  5
  6  H- |   7   3  10 |   6.99   3.00  10.02  |  0.022
  7
  8  H- |   5   8  15 |   4.99   7.99  15.00  |  0.016
  9  H- |   4  -8 -14 |   4.00  -8.03 -14.00  |  0.028
 10
 11
 12  H- |   7  -7   4 |   7.00  -7.00   4.00  |  0.003
 13  H- |   6  -6   2 |   6.01  -5.99   2.00  |  0.012
 14
 15  H- |   5  -7  -9 |   5.00  -6.99  -9.00  |  0.012
 16  H- |   7  -9  -4 |   7.00  -8.99  -4.01  |  0.016
 17  H- |   2  15  -4 |   2.00  15.01  -4.01  |  0.014
 18
 19  H- |   2   4 -16 |   2.00   3.99 -16.01  |  0.013
 20  H- |   2   5 -16 |   1.99   4.98 -16.00  |  0.026
 21  H- |   1  10 -10 |   1.00   9.99  -9.99  |  0.010
 22  H- |   1   8 -12 |   1.00   8.01 -11.99  |  0.018
 23
 24  H- |   1   4 -13 |   1.00   4.02 -13.00  |  0.025
 25  H- |   1   5 -12 |   1.00   5.00 -12.00  |  0.005
-------------------------------------------------------
  18h and  18H vectors out of  25.    Quality : 0.720

 Primitive cell :
                         9.590   20.375   22.889
                        73.67    89.99    89.95

 Volume of the cell  :     4291.67
```

Output of LePage.exe for solution no. 3 of example 7 (cf. solution no 2):

	LATO	LATT	A	B	C	ALFA	BET	GAM	VOL
INPUT CELL		P	9.590	20.375	22.889	73.67	89.99	89.95	4292.00
REDUC CELL		P	9.590	20.375	22.889	73.67	89.99	89.95	4292.00
CONV. CELL	M	P	20.375	9.590	22.889	90.01	106.33	89.95	4292.00