Auto-indexing program

- uses as starting input the previously stored list of 25 or less non-indexed reflections
- investigates the crystal without any further input about the crystal
- determines correct indices for these reflections
- calculates orientation matrix of the crystal
- does least-squares refinement of the matrix components
- calculates metrical tensor (Niggli matrix)
- determines normalized reduced unit cell
- prints pairs of perpendicular directions in direct lattice.

Matrix transformation program

- transforms unit cell and transformation matrix
- transforms orientation matrix
- transforms indices in reflection list on request
- saves transformation on specific file; old unit cell recalled by single command.

Reflection centering programs

- work with an input list of reflection positions, up to 25 reflections are possible
- use program controlled slits for fast running centering program
- produce an accuracy of centering which is better than 0.005° (this program is incorporated in the reflection search program and automatically centers the found reflections)
- prepare a new list of optimized reflection positions which are stored at same location as input list
- use the gravity center for optimization. This avoids $K\alpha_1/K\alpha_2$ split up problem
- contain special program provided to do additional, very accurate determination of 2θ value based on measurements at + and -2θ
- contain special program provided to do scan around any axis or combination of scans with print out of reflection profile and information about reflection centering
- achieve very accurate determination of cell constants and check alignment of the goniometer.

Orientation Matrix programs

- provide different starting input possibilities
  - calculate orientation matrix using unit cell parameters and 2 reflection positions

```
"
LS
 1  -1.001   2.000  -2.997   0.0361
 2  -1.001   1.997  -3.998   0.0337
 3  -3.000   1.998  -2.000   0.0239
 4  -1.002   0.999  -4.002   0.0320
 5  -3.001   1.001  -1.999   0.0300
 6  -2.001   0.998  -2.999   0.0377
 7   5.998  -0.002  -0.998   0.0225
 8   0.002   2.006   4.001   0.0700
 9  -0.001   6.000  -0.002   0.0198
10  -0.002  -6.002   0.001   0.0242
11  -0.003   0.998   6.003   0.0328
12   0.003  -1.000  -5.997   0.0271
13   0.000   1.994   8.002   0.0414
RECIPROCAL AXIS MATRIX
   0.082611   0.023330  -0.007429
  -0.052394  -0.035914  -0.091665
  -0.000895   0.077627  -0.001481

NIGGLI-VALUES
   148.1774   163.4779   157.8939
   -33.7179   -55.9565   -49.1129
 VOLUME=      1605.6960

CELL PARAMETERS
    12.1728    12.7858    12.5656
   102.1149   111.4587   108.3945
  -0.209869  -0.365829  -0.315555
"
DIRECT AXIS MATRIX
  11.510980   0.007187  -6.582241
  -0.870474  -0.207156 -10.330611
  -3.862276  12.784171  -2.801172

SIGMA DIRECT AXIS MATRIX
   0.003272   0.001364   0.002561
   0.005523   0.002303   0.004323
   0.003876   0.001616   0.003034

SIGMA CELL PARAMETERS
     0.0034     0.0035     0.0021
     0.0199     0.0206     0.0318
   0.000339   0.000335   0.000527
```