

Dirax

A.J.M. Duisenberg,
J. Appl. Cryst. (1992). **25**, 92-96.

help

- Typing “help” will open a webpage with the manual.
- Typing “help commandname” will open a webpage with the manual entry for the commandname.
Example: “help acl”

Important

- The program dirax will always give a primitive unit cell (P cell).
- The program “rmatrix” can be used to find higher metric symmetry (Bravais centering)

laboratory system

- Z-axis: rotation axis (“omega”)
- X-axis: direction from the crystal to the source
- Y-axis: completing the right-handed Cartesian system

rmat

- The rmatrix is build by the components of the reciprocal axes in columns
- x,y,z: laboratory system
- Note: This corresponds to the Nonius CAD4 definition

$$R = \begin{pmatrix} a_x^* & b_x^* & c_x^* \\ a_y^* & b_y^* & c_y^* \\ a_z^* & b_z^* & c_z^* \end{pmatrix}$$

Example

RMAT P

```
-0.15848170 -0.02721210 -0.03594000  
-0.09963430 -0.02403140 0.05858360  
0.06596800 0.19457920 0.00225960
```

TMAT P -3

```
1.00000000 0.00000000 0.00000000  
0.00000000 1.00000000 0.00000000  
0.00000000 0.00000000 1.00000000
```

```
SIGMA 0.00025 0.00134 0.00061 0.00811 0.00467 0.00416 0.05404
```

Note: The TMAT is applied to direct axis matrix (dmat)

Note2: The TMAT gives the possibility to save the Bravais centering and the point group.

Read drx-file

- With the command “read” you read the drx-file

go

- The command “go” starts the initial indexing.
- The column Acl contains a unique identifier for every indexing solution
- The column nH displays the number of indexed reflections
- The program automatically selects an Acl
- With the command “acl” the user can manually select an Acl

indexfit

- The command `indexfit` can be used to relax the criterion, if a reflection is considered indexed (H) instead of non-indexed (n)
- Remark: preferably used if indexing was already successful.

Example: indexfit 2

```
Dirax> acl
Acl  nH    a      b      c  alpha  beta  gamma  Volume S
186  12  3.255  3.786  4.267  92.91 101.15 110.98   48
185  24  3.244  3.787  4.254  92.76 100.90 111.19   47
183 208  5.804 14.535  5.819  90.02 119.80  89.98  426
182 194  5.805 14.541  5.820  89.99 119.80  89.92  426
181 202  5.805 14.541  5.820  90.00 119.81  89.93  426
180 206  5.807 14.539  5.824  89.94 119.83  89.99  427
178 208  5.806 14.541  5.823  89.97 119.81  90.00  427
174 196  5.807 14.554  5.825  90.09 119.83  90.02  427
172 202  5.806 14.540  5.820  89.99 119.81  89.95  426
169 209  5.806 14.539  5.823  90.02 119.81  90.01  426
166 199  5.806 14.542  5.820  90.00 119.82  89.93  426
165 208  5.807 14.542  5.824  90.03 119.82  90.02  427
157 202  5.806 14.540  5.821  90.00 119.81  90.04  426
156 206  5.806 14.540  5.821  90.00 119.81  90.03  426
151 207  5.807 14.541  5.822  89.98 119.82  89.98  427
146 202  5.804 14.539  5.821  90.00 119.79  90.03  426
141 199  5.803 14.533  5.818  90.02 119.82  90.03  426
140 202  5.804 14.535  5.819  90.00 119.81  89.98  426
138 203  5.803 14.534  5.818  90.01 119.80  89.98  426
124 184  5.800 14.521  5.815  89.94 119.82  89.98  425
 46 184  5.801 14.520  5.815  89.92 119.82  89.98  425
 35 184  5.801 14.522  5.816  89.93 119.81  89.98  425
 28  35  1.942  4.889  5.126  88.57  79.36  82.39   47 ?
 27  35  3.550  4.159  4.182  88.25  82.54  82.68   61
 25  25  3.526  4.167  4.177  88.27  82.70  82.61   60
 18   7  1.627  4.293  4.867 101.67  90.90  99.52   33 ?

169 209  5.806 14.539  5.823  90.02 119.81  90.01  426
acl/auto [169] 
```

Example: indexfit 4

```
Dirax> indexfit 4
Dirax> acl
Acl  nH  a      b      c  alpha  beta  gamma  Volume S
186  53  3.242  3.783  4.251  92.80  100.87  111.24  47
183  445  5.806  14.545  5.815  90.00  119.82  90.07  426 Q
182  446  5.806  14.546  5.815  89.98  119.82  89.92  426 Q
181  447  5.806  14.546  5.816  90.02  119.82  90.08  426 Q
180  443  5.807  14.547  5.816  89.96  119.83  89.96  426 Q
178  445  5.807  14.545  5.817  89.96  119.83  89.97  426 Q
174  449  5.806  14.549  5.816  89.97  119.82  89.93  426 Q
172  449  5.806  14.548  5.817  90.03  119.82  90.09  426 Q
169  442  5.806  14.543  5.818  90.04  119.83  90.02  426 Q
166  450  5.806  14.552  5.816  90.02  119.81  90.09  426 Q
165  442  5.807  14.547  5.817  90.03  119.83  90.04  426 Q
157  439  5.806  14.546  5.816  89.98  119.82  89.95  426 Q
156  441  5.807  14.546  5.818  89.97  119.83  89.96  426 Q
146  447  5.806  14.544  5.815  90.01  119.82  90.07  426 Q
141  446  5.806  14.543  5.815  90.01  119.82  90.07  426 Q
140  443  5.806  14.544  5.815  89.98  119.82  89.95  426 Q
124  445  5.805  14.543  5.815  90.01  119.82  90.07  426 Q
 46  446  5.805  14.544  5.815  90.01  119.82  90.07  426 Q
 28  57  1.941  4.894  5.124  88.51  79.34  82.50  47 ?
 27  75  3.551  4.165  4.179  88.23  82.49  82.75  61
 25  75  3.550  4.166  4.179  88.24  82.46  82.76  61
 18  44  1.631  4.285  4.864  101.42  90.54  99.82  33 ?

 27  75  3.551  4.165  4.179  88.23  82.49  82.75  61
acl/auto [27] 166
```

levelfit

- Relax criterion if a reflection is considered indexed (H) instead of non-indexed (n)
- Remark: preferably used, if indexing fails

store

- Stores indexing solution in internal memory

Ichi

- Inverts current index status:
 - indexed (H) becomes non-indexed (n)
 - non-indexed (n) becomes indexed (H)

compare

- Compares different indexing solutions
- Example:
compare a b
(compares solution a with solution b)

savermat

- The command “savermat” writes the indexing solution (rmat) into file