

tCorient

SBC01-????-00

June 29, 1995

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TABLE OF CONTENTS

1 SCOPE AND PURPOSE	3
1.1. Definitions and Abbreviations	3
2 BACKGROUND	3
3 INPUT IMAGE	4
4 RUNNING TCORIENT	6
4.1. Example.....	9
4.2. Overcoming difficulties.....	10
5 FILE FORMATS	11

1 Scope and Purpose

This document describes how to use the tCorient module of d*TREK. tCorient tests the crystal orientation module of d*TREK. It serves as an aid in orienting a crystal for a specific data collection strategy. For example, the crystal may be oriented so that a mirror plane is perpendicular to a rotation axis. In such an orientation, Bijvoet pairs can be collected simultaneously on an area detector.

1.1 Definitions and Abbreviations

The definitions described in the dtpredict and tCrefine documents are appropriate for tCorient

2 Background

In a single crystal diffraction experiment, the crystal is often mounted randomly on the crystal goniometer. Only after finding the centroids of a few Bragg reflections with dtfind and indexing them with tCindex is the crystal orientation known. A random crystal orientation may not be the best for data collection. In combination with a 3-circle crystal goniometer, tCorient allows one to orient the crystal so that a specific data collection strategy can be used. Three examples of a specific orientation are described next.

In order to reduce systematic differences between anomalous pairs F^+ , F^- it is desirable that these pairs be collected simultaneously on a detector. To do this, a crystal mirror plane must be oriented perpendicular to the data collection rotation axis. tCorient can calculate the goniometer angles to satisfy this condition.

In order to collect complete datasets, a simple strategy is to rotate the crystal around a principal crystal axis, then rotate around a second axis to get reflections that were in the blind region. When the crystal is rotated around an axis, it is important that the rotation begin and end at optimal angles. For example, in an orthorhombic system, the crystal must be rotated through 90° to get fairly complete data, but the 90° should start at one mirror plane and continue to the next. If the rotation begins 45° from a mirror plane, then reflections in the range $0-45^\circ$ will be symmetrically equivalent to reflections in $45-90^\circ$ with the result that the dataset will be less than 50% complete. tCorient can calculate the goniometer angles so that the rotation spans the correct 90° range.

In situations where multiple crystals must be used to collect a final complete merged dataset, it is important that there are common reflections between the datasets from

different crystals but the datasets do not completely overlap so that the overall completeness can approach 100%. With randomly oriented crystals, there is a chance that a lot of redundant data is collected without getting 100% completeness. tCorient can orient each crystal in a specific way, such that data collection on a subsequent crystal picks up where it finished on the previous crystal.

tCorient uses a vectorial description of the crystal, source, detector and their goniometers. This vectorial description has been described in the *dtpredict* document, in the *Proceedings of the EEC Cooperative Workshop on Position-Sensitive Detector Software (Phases I & II)*, *ibid. (Phase III)*, and in *Computational Aspects of Protein Crystal Data Analysis DL/SCI/R25*. The reader is referred to these documents for a complete description.

3 Input image

tCorient requires one image as input. It reads the header of the input image to get the initial values of the source, crystal, and crystal goniometer properties. tCorient does not need to read the binary pixel data in the image which may be even be missing (i.e. the image is dimensioned 0 by 0). A typical image header is shown below. The keywords required by tCorient are limited to those describing the crystal, the crystal goniometer and the source. These are shown in bold below. It does not use keywords required for the detector. Keywords are described in the *dtpredict* documentation.

```
1 {
2  HEADER_BYTES= 2048;
3  TYPE=mad;
4
5  SIZE1=0;
6  SIZE2=0;
7  SCAN_TITLE=start end inc time nOsc nDark nDup nDlim nDC nDCup;
8  SCAN_ROTATION=0.0 12.0 0.2 4 0 1 0 100 1 0;
9  SCAN_ROTATION_AXIS_NAME=omega;
10 SCAN_ROTATION_VECTOR=1.0 0.0 0.0;
11 SCAN_TEMPLATE=test3.####.ss;
12 SCAN_SEQ_INFO=0 2 0;
13 ROTATION=0.0 0.2 0.2 4 0 1 0 100 1 0;
14 ROTATION_VECTOR=1.0 0.0 0.0;
15 ROTATION_AXIS_NAME=omega;
16 CRYSTAL_MOSAICSPREAD=0.145;
17 CRYSTAL_DESCRIPTION=Test of tCorient;
18 CRYSTAL_REFINE_FLAGS=0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
19 CRYSTAL_ORIENT_VECTORS=1 0 0 0 1 0 0 0 1;
20 SOURCE_VECTORS=0.0 0.0 1.0 0 1 0 1 0 0;
21 SOURCE_POLARZ=0.5 1.0 0.0 0.0;
22 SOURCE_SPECTRAL_DISPERSION=0.0002 0.0002;
23 SOURCE_SIZE=0.0 0.0 0.0 0.0;
```

```
24 SOURCE_CROSSFIRE=0.0 0.0 0.0 0.0;
25 SOURCE_WAVELENGTH=1 1.54178;
26 SOURCE_REFINE_FLAGS=0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
27 DETECTOR_NUMBER=1;
28 DETECTOR_NAMES=D0_;
29 D0_NONUNF_TYPE=Dark_only;
30 D0_NONUNF_INFO=nonunf.img dark.img;
31 D0_SPATIAL_DISTORTION_TYPE=Interp_spatial;
32 D0_SPATIAL_DISTORTION_INFO=distor;
33 D0_DETECTOR_DIMENSIONS=512 512;
34 D0_DETECTOR_SIZE=50.0 50.0;
35 D0_DETECTOR_VECTORS=1 0 0 0 1 0;
36 D0_DETECTOR_DESCRIPTION=ANL-SBC gold detector single module;
37 D0_DETECTOR_REFINE_FLAGS=0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
38 D0_GONIO_NUM_VALUES=6;
39 D0_GONIO_NAMES=RotZ RotX RotY TransX TransY TransZ;
40 D0_GONIO_UNITS=deg deg deg mm mm mm;
41 D0_GONIO_VECTORS=0 0 1 1 0 0 0 1 0 1 0 0 0 1 0 0 0 -1;
42 D0_GONIO_VALUES=1.0 2.0 0.0 -.5 -.8 102.3;
43 D0_GONIO_DESCRIPTION=A simple detector goniostat;
44 CRYSTAL_GONIO_NUM_VALUES=3;
45 COMMENT=Header edited by dtheadredit;
46 CRYSTAL_UNIT_CELL=79.2 79.2 38.9 90. 90. 90;
47 CRYSTAL_ORIENT_ANGLES= 10.000 20.000 30.00;
48 CRYSTAL_SPACEGROUP=96;
49 CRYSTAL_GONIO_NAMES=Omega Chi Phi;
50 CRYSTAL_GONIO_UNITS=deg deg deg;
51 CRYSTAL_GONIO_VECTORS=1.000 0.000 0.000 0.000 0.000 1.000 -1.000
0.000 0.000;
52 CRYSTAL_GONIO_DESCRIPTION=A 3-circle eulerian crystal goniostat;
53 CRYSTAL_GONIO_VALUES=10.000 -23.294 134.937;
54 FILENAME=lyso3.img;
55 BYTE_ORDER=big_endian;
56 Data_type=short int;
57 COMPRESSION=None;
58 }
```

4 Running tCorient

After tCorient has been installed and placed in your PATH, just enter tCorient. This version takes no command line options, but instead prompts for an image file name. It reads the image header along with any binary image data in the file. Messages are written to stdout and stderr as required. It prompts for an orientation request which it tries to fulfill. The user chooses from a number of possible solutions to the request. Finally, the name of an output image file is requested. A file with a new header that contains the selected result is written. The syntax for running tCorient is:

```
tCorient
```

The program will list the angles between the six principal crystal vectors: **a***, **b***, **c***, **a**, **b**, **c** and seven laboratory vectors: **source**, the goniometer axes (i.e. **omega**, **chi**, **phi**), and lab **x**, **y**, **z**. The angles are calculated for when the crystal goniometer is at the position described by the CRYSTAL_GONIO_VALUES keyword. This position is sometimes called the home, zero or datum position. These are the goniometer values when the crystal is rotated by 0° around the data collection rotation axis. The angles are presented in tabular form:

1	Orient listing						
2	When the crystal goniometer is at:			10	-23.294	134.94	
3	the angles between crystal vectors and lab vectors are:						
4			Crystal vectors				
5		a*	b*	c*	a	b	c
6	Lab vectors:						
7	Source	103.71	141.21	125.44	103.71	141.21	125.44
8	Omega	58.635	127.29	53.009	58.635	127.29	53.009
9	Chi	95.222	137.73	131.79	95.222	137.73	131.79
10	Phi	144.47	63.834	112.24	144.47	63.834	112.24
11	Lab X	58.635	127.29	53.009	58.635	127.29	53.009
12	Lab Y	145.12	99.158	56.678	145.12	99.158	56.678
13	Lab Z	103.71	141.21	125.44	103.71	141.21	125.44

In the above listing, the crystal appears to be randomly oriented. Note that the angles between the crystal and the 'Source' and 'Lab Z' are identical because the source is pointed along laboratory Z. Likewise, 'Omega' and 'Lab X' are the same axis.

Next, tCorient prompts for an orient request:

```
Enter orient request:
```

The request takes one of two forms. The first form is a string which contains two crystal vector, laboratory vector pairs. The second form is a string which begins with the word 'rot' followed by an angle in degrees and a vector description.

Form 1: **crys1 || lab1; crys2 || lab2**

The crystal vector and laboratory vector in each pair is separated by the || characters which denote that the crystal vector should be made parallel to the laboratory vector. The first pair is separated from the second pair by a semicolon. A crystal vector can be the name of a principal crystal axis, an hkl (a direction in reciprocal space), a vector along the real cell axes, or a vector along crystal orthogonal axes.

The supported names of principal crystal axes are:

a b c -a -b -c a* b* c* -a* -b* -c*

An hkl is three numbers enclosed in parentheses:

(1 1 0)

A vector along the real cell axes is three number enclosed in square brackets:

[1.5 1 0]

A vector along orthogonal axes is either the axis name

x y z -x -y -z

or three numbers without the parentheses or square brackets:

1.5 2.0 0.75

The laboratory vector can be the name of a principal laboratory axis, the source, the first crystal goniometer axis defined by the input image header or 3 numbers.

The supported names of principal laboratory axes are:

x y z -x -y -z

The source vector is simply

source -source

The first goniometer axis can be specified either by its name or the word gon1:

omega -omega gon1 -gon1

A general laboratory vectors is specified by three numbers without the parentheses or square brackets:

1.5 2.0 0.75

Note that $a^* = (1\ 0\ 0)$, $-a^* = (-1\ 0\ 0)$, $b = [0\ 1\ 0]$, etc.

Here are several examples (note the ; to separate pairs!):

a* || source; b* || omega
a* || source; b* || x

```
(1 1 0) || x; b*|| -y
a* || z; b*|| 1 1 0
a* || -y; b*|| omega
```

These examples are invalid:

```
a* || source
```

Only one pair is given.

```
a* || source b*|| omega
```

The semicolon is missing.

```
c || chi; b*|| x
```

Chi is not the first goniometer angle.

tCorient will calculate goniometer angles which make the first crystal vector parallel to the first laboratory vector and the second crystal vector will be in the plane formed by second laboratory vector and the first laboratory vector if this is possible. Thus the order of the crystal vector || laboratory vector pairs is important. For a monoclinic b-axis unique cell the following are not the same:

```
a* || source; b*|| omega
b* || omega a*|| source
```

If the requested orientation is not possible this will be reported. Here is an example of a request that cannot be fulfilled:

```
a* || source; b*|| source
```

Form 2: rot degs lab1

This form is used to rotate the crystal around a virtual laboratory axis which usually does not coincide with a crystal goniometer axis. Simply enter the word `rot` followed by a relative angle to rotate by and a vector to rotate around. Positive rotations are right-handed. The vector may be left off the request which then defaults to `source`. Otherwise, the vector is a laboratory vector as described in the previous section. Here are some examples:

```
rot 50
rot 45 x
rot 60 -y
rot -30 1 1 0
```

Which directions are laboratory X, Y, Z?

Since d*TREK and tCorient make use of a vectorial notation, different laboratory reference frames may be used at different installations. A laboratory reference frame is usually chosen by how the source vector and the first goniometer axis vectors are chosen. See the note at the end of the first listing in this section for an example.

4.1 Example

```
1  tOrient
2  Enter name of image to get crystal and goniometer info from:
   lyso3.img
3      File lyso3.img successfully opened.
4      Header of file lyso3.img successfully read.
5      Image is 0 by 0 pixels.
6      Data_type in header is short int.
7      Compression_type is None.
8      Byte_order is big_endian.
9      WARNING in Cimage:nRead, data size is <= 0.

10 Orient listing
11 When the crystal goniometer is at:          10  -23.294  134.94
12 the angles between crystal vectors and lab vectors are:
13                                     Crystal vectors
14                                a*      b*      c*      a      b      c
15 Lab vectors:
16 Source  103.71  141.21  125.44  103.71  141.21  125.44
17 Omega   58.635  127.29  53.009  58.635  127.29  53.009
18 Chi     95.222  137.73  131.79  95.222  137.73  131.79
19 Phi    144.47  63.834  112.24  144.47  63.834  112.24
20 Lab X   58.635  127.29  53.009  58.635  127.29  53.009
21 Lab Y   145.12  99.158  56.678  145.12  99.158  56.678
22 Lab Z   103.71  141.21  125.44  103.71  141.21  125.44
23
24 Enter orient request: a||omega; b||source
25
26 Solutions to orient:
27 Solution  Omega      Chi      Phi
28 0          10      -23.294  134.94  <- Current goniometer zero
29 1          49.358  324.47  -36.052
30 2         -130.64  35.531  143.95
31 3         -49.358  215.53  143.95
32 4          130.64  144.47  -36.052
33 5         -130.64  324.47  -36.052
34 6          49.358  35.531  143.95
35 7          130.64  215.53  143.95
36 8         -49.358  144.47  -36.052
37 Enter the number of the selected solution: 6
38
39 Orient listing
40 When the crystal goniometer is at:          49.358  35.531  143.95
41 the angles between crystal vectors and lab vectors are:
42                                     Crystal vectors
43                                a*      b*      c*      a      b      c
44 Lab vectors:
45 Source   90      180      90      90      180      90
46 Omega    0       90      90      0       90      90
47 Chi     90     130.64  139.36  90     130.64  139.36
48 Phi    144.47  63.834  112.24  144.47  63.834  112.24
```

```
49      Lab X      0      90      90      0      90      90
50      Lab Y      90      90      0      90      90      0
51      Lab Z      90     180     90      90     180     90

52 Enter name of image output file to write with results: lyso3out.img
53 File lyso3out.img successfully opened.
```

Explanation

- Line 1 **tCorient** is started.
- Line 2 The input image file is requested and the name is typed in.
- Lines 3-9 Information about the image file is listed.
- Line 9 This image file has no data -- just a header.
- Lines 10-22 The angles between crystal axes and several laboratory axes are listed.
- Line 24 The orientation request is given: the crystal **a** axis should be parallel to the omega axis and the crystal **b** axis should be parallel to the source.
- Lines 26-37 Eight different solutions are calculated. There are eight since **tCorient** gives valid solutions that are 180° apart.
- Line 35 Solution 6 is selected.
- Lines 39-51 The new angles between the crystal axes and several laboratory axes are listed. Note that the angle between the crystal **a** axis and omega is 0 and the angle between the crystal **b** axis and the source is 180. Thus the request was fulfilled.

4.2 Overcoming difficulties

Since **tCorient** gets all of its input information from an image header, difficulties may arise when the header is incomplete. Be especially careful that the crystal goniometer vectors are described properly and in the correct order in the header. The first crystal goniometer axes is closest to the baseplate, the last crystal goniometer axis is closest to the crystal. If the crystal goniometer does not have 3 axes, then **tCorient** cannot function properly. It is meant to be used with a 3-circle crystal goniometer.

The output of tOrient clearly shows when any files have not been read properly. Examine the output to ensure that the header has been read correctly. If not, then the image header is incorrect and should be modified.

In these cases, add or correct the information (use dtheadredit, see section 5 of the dtpredict manual) and run tOrient again.

If the requested orientation cannot be achieved, then the 'Usage' text below will be output. Check that the request specifies two different crystal vectors and two different laboratory vectors.

```
1  No solutions available.
2  Usage:
3  -EITHER-
4    crystal_vector1 || lab_vector1; crystal_vector2 || lab_vector2
5  where
6  crystal_vector is one of
7    a, b, c, -a, -b, -c, a*, b*, c*, -a*, -b*, -c*, (h k l), [r s t]
8    (h k l) is a Miller index, while [r s t] is a real direction
9                                     along real unit cell axes;
10 lab_vector is one of
11    x, y, z, -x, -y, -z, source, -source, gon1, -gon1, xl yl zl
12    gon1 is the name of the first goniometer axis (i.e. omega)
13    xl yl zl is a sequence of 3 numbers.
14  -OR-
15    rot fAngle lab_vector
16  where
17  rot is the word rot
18  fAngle is a relative amount to rotate in degrees
19  lab_vector is described above and defaults to source if missing.
```

5 File formats

Image file formats are discussed in the `calibrate` and `dtpredict` documentation. An example of an image header is given in Section 3.