MHATT-CAT's Newport Kappa Diffractometer
Version 2.32

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Abstract

This is a user manual for MHATT-CAT's Newport/Microcontrole kappa-style "psi-circle" diffractometer, also known as a General Purpose Diffractometer, located in the 7-ID-C hutch of the APS. Some of the content may be generally applicable to various diffractometers, but some is specific to MHATT-CAT's kappa. This document will probably always be a work in progress; comments, questions, and suggestions are always welcome.

Contents

1 Introduction

This document describes some of the aspects of using the Newport/Microcontrole psi-circle kappa-style diffractometer located in hutch 7-ID-C of MHATT-CAT. The psi-circle geometry has six rotation axes, but is distinguished from the standard “six-circle” diffractometer by the arrangement of detector circles. A psi-circle diffractometer is also known as “4S+2D,” after the four sample-orientation axes and two detector-orientation axes; the sample and detector move independently. The angle calculations for this diffractometer were worked out by Hoydoo You of MSD, Argonne [1]. The kappa geometry was invented by Poot for Enraf-Nonius [2] and is described in detail by Sands [3] and Robinson [4]. The kappa geometry has significant advantages over the traditional Eulerian geometry (i.e., the geometry with the chi circle), but certainly takes time to get used to. Mathematical transformations can be used to switch between kappa and Eulerian geometries, and are discussed below in detail.

The Newport kappa (as the diffractometer is often referred) uses servo motors (and some stepper motors, for linear motions) controlled by Newport MM4005 motor drivers. The motors are moved through EPICS (or directly via the front panel of the MM4005 driver). Diffractometer calculations are performed by SPEC, either with four circles in the “kappa” geometry or all six circles in the “psic” geometry. This brief manual will describe some of the features of this diffractometer and its control via SPEC [5]. Information common to all SPEC geometries (such as setting up an orientation matrix) is generally not included. The psic and fourc help files in SPEC may provide additional help.

MHATT-CAT’s Newport kappa is located toward the downstream, inboard corner of the 7-ID-C hutch. The MM4005 motor controllers are on a short, enclosed equipment rack inside the hutch. The upper MM4005 controls the six rotation axes, while the lower MM4005 controls the five table motors and three sample stages. The large red button on the front of the rack turns off power to the rack (and, correspondingly, to the diffractometer); if this button is pushed, all motor positions are lost and need to be re-homed. To protect the diffractometer from collisions, several sets of optical limit switches are placed at various locations, such as the detector arm and the upstream pillar. There are also two red buttons connected to the control rack via BNC cables; these panic buttons are equivalent to the optical limit switches and will turn off power to the motors but not to the motor drivers. Typically, one button is located inside the hutch, one outside at the 7-ID-C control computer.

2 Angles, Motors, and Pseudomotors

The Newport kappa diffractometer has six motors for sample and detector orientation. Two SPEC geometry codes are available for controlling the diffractometer: kappa, to operate four circles (not moving the vertical axes), and psic, to operate all six circles. It is possible in both SPEC geometries to make a transformation between the "real motors" (i. e., motors which are physically present on the diffractometer) of kappa geometry and the "pseudomotors" of Eulerian geometry. That is, the diffractometer can operate just as if there is a chi circle. Operation in Eulerian geometry can be somewhat transparent to the user (although one must be particularly careful about collisions), yet can be confusing for someone not used to the kappa geometry. The kappa transformations are discussed in more detail in Section 2.3.

2.1 Angle nomenclature

Unfortunately, there are different conventions for naming the motors of the diffractometer (Newport's convention vs. kappa's vs. psic's). This is a problem since the names of real motors in some conventions are the names of pseudomotors in other conventions! Table 1 attempts to sort out the various names of motors and pseudomotors, and Table 2 lists some other angles which are important in SPEC. Fig. 1 defines the psi-circle angles in Eulerian geometry.

EPICS name	SPEC name		Comments
	kappa	psic	
Real Motors			
2-theta	tth	del	horizontal axis for detector arm
Omega	kth	keta	horizontal axis for sample (kth/keta short for k-theta/k-eta)
Kappa	kap	kap	sample motor
Phi	kphi	kphi	sample motor
Nu	N/A	nu	vertical axis for detector, only for psic
Psi	N/A	mu	vertical axis for sample, only for psic
Pseudomotors			
N/A	th	eta	the Eulerian theta/eta
N/A	chi	chi	range limited by kappa geometry: $-100° < \text{chi} < 100°$
N/A	phi	phi	the Eulerian phi

Table 1: The many different ways to name diffractometer motors.

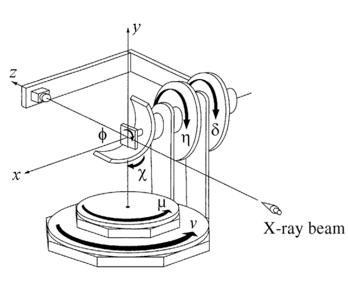

Figure 1: Basic definition of (Eulerian) psi-circle diffractometer angles, from Ref. [1]. Of course, the chi circle is merely a "pseudomotor" on a kappa diffractometer. The physical detector arm (and the delta motor) are on the opposite side of the figure; thus, the rotation senses described in the figure represent the positive motion of the detector but not of the physical motor delta.

Common to kappa and psic	
F_*XYZ*	frozen value of angle *XYZ* for fixed-*XYZ* modes (*XYZ* = ALPHA, DEL, etc.)
CUT_*XYZ*	cut point of motor *XYZ* (see sections 3.1.3 and 3.2.3)
g_kappa	the mechanical angle of the kappa arm relative to the kth/keta axis (about 50°). Sometimes known as α or $\alpha_\circ$.
Specific to kappa	
alpha	incident angle (if reference vector is surface normal)
beta	exit angle
omega	th-tth/2
azimuth	rotation angle of reference vector about Q
Specific to psic	
tth	total scattering angle, a function of del *and* nu
alpha	incident angle (if reference vector is surface normal)
beta	exit angle
psi	azimuthal angle of the reference vector with respect to Q and the scattering plane
tau	longitudinal angle of the reference vector with respect to Q and the scattering plane
Qaz	azimuthal angle of scattering vector Q
Naz	azimuthal angle of the reference vector
omega	angle between Q and the chi-circle
sigma_az	the chi part of the azimuthal angle specification (see Sect. 3.2.3)
tau_az	the phi part of the azimuthal angle specification (see Sect. 3.2.3)

Table 2: Various angular parameters for SPEC geometries. Q is the diffraction vector, with $|Q| = 2\sin(2\theta/2)/\lambda$. See Sects. 3.1.2 and 3.2.2 on how to define the reference vector.

2.2 Setting motor positions

Sometimes one can set a motor position in SPEC with the `set` command, such as
`set tth 5`
However, you cannot set the value of a pseudomotor the same way, e. g.,
`set th 5`
It won't work! There is no motor to set a value to! It is also a bad idea even to set real motors to arbitrary values; it will only lead to confusion and problems when calculating pseudomotor positions. For example, if you find a symmetric Bragg reflection at tth = 20 and th = 10.5, you may be tempted to set kth to 10 since you "know" that is where the reflection should be. Please don't do it!

2.3 Eulerian-kappa transformations

The mathematical transformations between Eulerian and kappa geometries are shown in Eq. 1 and 2, where $\alpha_\circ$ = g_kappa is the tilt angle of the kappa arm. The design value of $\alpha_\circ$ was 50° and the angle was recently measured to be 49.96°. To transform from Eulerian to kappa geometry,

$$\begin{aligned} \text{kth} &= \text{th} - \arcsin[-\tan(\text{chi}/2)/\tan(\alpha_\circ)], \\ \text{kap} &= 2\arcsin[\sin(\text{chi}/2)/\sin\alpha_\circ], \\ \text{kphi} &= \text{phi} - \arcsin[-\tan(\text{chi}/2)/\tan(\alpha_\circ)]. \end{aligned} \tag{1}$$

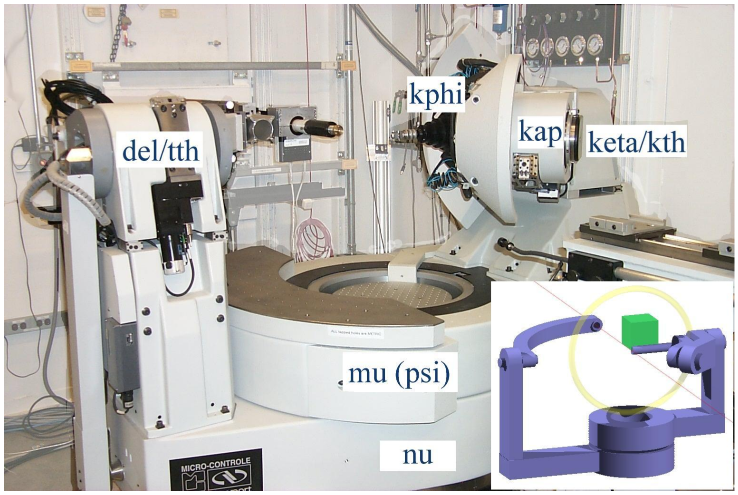

Figure 2: Newport kappa in 7-ID-C with all motors at 0°, before being rotated. Real motors are labeled (psic geometry names followed by kappa names, where they differ). Inset: Diagram of the motors at 0°, from a slightly higher point of view than the photograph. The red line is the direction of the direct beam, and the yellow circle represents the full chi arc.

To transform from kappa to Eulerian geometry,

$$\begin{aligned} \text{th} &= \text{kth} - \arctan[\tan(\text{kap}/2) * \cos(\alpha_\circ)] = \text{kth} - \cos(\text{kap}/2)/\cos(\text{chi}/2), \\ \text{chi} &= 2\arcsin[\sin(\text{kap}/2) * \sin\alpha_\circ], \\ \text{phi} &= \text{kphi} - \arctan[\tan(\text{kap}/2) * \cos(\alpha_\circ)] = \text{kphi} - \cos(\text{kap}/2)/\cos(\text{chi}/2). \end{aligned} \tag{2}$$

For the psic geometry code, replace th and kth with eta and keta, respectively. These transformations are found in the s4c_to_ka and ska_to_4c functions in the geo_fourc.c file; note that SPEC no longer maintains separate geometry files for kappa-type diffractometers. These conversions have also been implemented on a MHATT-CAT web page [6].

A couple of tricks are used in SPEC's configuration file to keep track of these motors. Some real motors have different names in the different geometries, so instead of being entered in config once in the "common" geometry, they are entered separately for each geometry with the appropriate name. Since EPICS keeps track of all the motor settings (position, steps/degree, etc.) there is no potential problem of changing the settings in one geometry but not having the other geometry be updated. All the pseudomotors have motor type "NONE" in config, so SPEC knows there is no physical motor associated with that name. The resolution (steps/deg) of the pseudomotors should be set rather high to avoid round-off errors when pseudomotor positions are displayed.

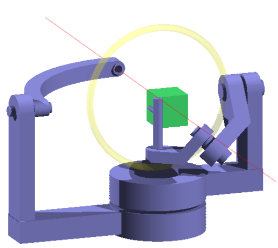

Figure 3: Diagram of a kappa psi-circle diffractometer with all pseudomotors at 0° except chi = 90°. Note that three real motors (kth/keta, kap, and kphi) have moved relative to Fig. 2 in order to move one pseudomotor.

3 SPEC Geometries

To reach a given $hk\ell$ point in reciprocal space, for example, using the `br` command, the diffractometer's angles must be moved to certain positions. But there are, in general, ambiguities which must be addressed in order to choose those positions. There are three sources to those ambiguities, which SPEC resolves via the user's selection of *modes*, *sectors*, and *cut points*. Since there are some differences between the kappa and psic geometries in how these selections are made, they are addressed separately. The current state of all the settings described in this section can be checked with the `pa` command.

3.1 kappa

3.1.1 Modes

The general issue in transforming from reciprocal space to diffractometer angles in kappa geometry is that there are three constraints (the Miller indices h, k, and ℓ) but four variables (the angles tth, kth, kap, and kphi). Thus one additional constraint is needed to lift this degeneracy and uniquely determine the diffractometer angles; SPEC calls this constraint a *mode*. A mode is selected with the `setmode` command; type
`setmode` *value*
to select mode *value*, or just type
`setmode`
to see the available modes. Table 3 lists the seven modes in four-circle geometry.

Each mode requires an angle (or two) to be fixed. The fixed value(s) can be chosen with the `freeze` command. In a given mode, typing
`freeze` *value*
will freeze whatever angle is to be fixed, at *value* (two values are needed for mode 2). Leaving off *value* will freeze the appropriate angle at its current position (and leave the angle fixed there); you won't be prompted for a value. In frozen mode, the constraint will be used regardless of the current diffractometer position. The command
`unfreeze`
will calculate modes based on the current position of the appropriate angle. If the relevant angle is moved (by the command `umv`, for instance), then the calculation will yield a different result (unlike frozen mode).

Mode	Description	Frozen variable	Comments
0	Omega equals zero	—	simplest case; special case of mode 1
1	Omega fixed	F_OMEGA	
2	Zone	F_CHI_Z,	chi and phi fixed; can only reach a plane of reciprocal
		F_PHI_Z	space (use `cz`, `pl`, `mz`, and `sz` commands)
3	Phi fixed	F_PHI	three-circle geometry
4	Azimuth fixed	F_AZIMUTH	fix azimuth at ±90 for alpha = beta
5	Alpha fixed	F_ALPHA	typically the incidence angle
6	Beta fixed	F_BETA	typically the exit angle

Table 3: Modes in kappa geometry.

3.1.2 Azimuth

Selecting the azimuth essentially means picking a reference direction on the sample. This direction could be the surface normal, magnetic field direction, etc. In kappa geometry it is only chosen by Miller indices. Type
`setaz` $h\ k\ \ell$
to give the Miller indices (the vector's magnitude, of course, does not matter), or just
`setaz`
to be prompted for its indices one at a time.

3.1.3 Sectors and cut points

In addition to the constraint provided by the choice of mode, there are further ambiguities in the selection of angles to reach a given $hk\ell$. As a somewhat trivial example, the set of angles (tth,th,chi,phi) of (40,20,0,0) has the exact same diffraction condition as does (-40,160,0,0), but usually one wants to diffract upwards, not downwards. SPEC is told how to resolve this type of ambiguity through *sectors*.

There are eight symmetry transformations which lead to equivalent diffraction conditions; these are labeled as sectors 0 to 7. I will not reprint them here, but they are listed in SPEC's online help file (under "fourc"). To choose a sector, use the command
`setsector` *value*
to choose sector *value*, or leave off *value* to be prompted for it. More usefully, you can see all the possible sets of angles for a given reciprocal lattice point using the command
`sectors` $h\ k\ \ell$.
This command will list alpha, beta, azimuth, omega, and the Eulerian angles for all possible sectors (only sectors 0 through 3 are available to modes 4, 5, and 6). Remember that $|\text{chi}| \leq 100$ is required by kappa geometry; an error message appears when the pseudo-to-real motor transformation cannot be made.

The final ambiguity is due to the 360° periodicity of the circle: the angle of $-10°$ is equivalent to 350°, but if you are currently at $+5°$, you probably want to move down by 15° instead of up by 345°. *Cut points* are used to tell SPEC where to divide the circle. An angle with a cut point of x will move between x and $360{+}x$. Cut points of the seven real and pseudomotors are set with the command `cuts`. Typing
`cuts`
will prompt the user for the cut points of the seven real and pseudomotors. Alternately, one can type
`cuts` *angle value*
to set the cut point of a particular *angle*. The SPEC helpfile is not quite up-to-date on cut points. Typically, cut points at -180 are fine for most motors, but it's better to use -170 for th/kth (or eta/keta), since the real motor has a range of 540°.

3.2 psic

3.2.1 Modes

Selecting a mode in psic geometry is considerably more complicated than in kappa geometry, since three constraints must be added to the three Miller indices to uniquely determine all six angles. Unlike SPEC's sixc code, which "features" an ever-lengthening list of modes to choose from, psic's mode selection is based on a table formalism. That is, up to five variables (g_mode1, g_mode2, ... g_mode5) select the mode according to Table 4. Although this formalism may be confusing, it

psic	g_mode1	g_mode2	g_mode3	g_mode4	g_mode5
0	·	·	··· omega-fixed ···		X
1	delta-fixed	alpha=beta	······ eta-fixed ······		
2	nu-fixed	alpha-fixed	······ mu-fixed ······		
3	qaz-fixed	beta-fixed	······ chi-fixed ······		
4	naz-fixed	psi-fixed	······ phi-fixed ······		
5	Zone	X	eta=del/2	X	X
6	X	X	mu=nu/2	X	X

Table 4: Table to select modes in psic geometry, from SPEC's psic helpfile and Ref. [1]. Entries with X are not used.

allows for, in principle, a very general selection of angular constraints. But beware that some sets of constraints have not had geometry code written or fully debugged.

To select a mode in psic geometry, the general format is
`setmode` *g_mode1 g_mode2 g_mode3 g_mode4 g_mode5*
where *g_modeN* = 0 to 6, although you often don't need to specify all five numbers each time. Generally, g_mode1 refers to a detector angle constraint, g_mode2 to an azimuthal angle constraint, and g_mode3 thru g_mode5 to sample angle constraints. Here are several examples of mode selection.

These three modes can imitate a four-circle diffractometer, if `F_NU=0` and `F_MU=0`:

- `setmode 2 1 2` chooses alpha=beta
- `setmode 2 2 2` choose alpha
- `setmode 2 3 2` choose beta

Typical surface diffraction modes:

- `setmode 4 1 5`
- `setmode 4 2 5` For these modes, `F_NAZ=0` keeps the surface normal horizontal, and rod scans are done by rocking phi (chi stays near zero). But it may be better to operate with `F_NAZ` in the range of 5 to 15 (12 is often used) to avoid cut-point type issues.

Horizontal or vertical scattering:

- `setmode 3 1 5` `F_QAZ=0` keeps the diffraction vector Q horizontal.
- `setmode 3 1 6` `F_QAZ=90` keeps the diffraction vector Q vertical.

Zone mode:

- `setmode 5` chi and phi are chosen to keep Q in a chosen plane, using the macros `sz`, `cz`, and `mz`.

Other general modes:

- `setmode 0 0` *s1 s2 s3* Three sample angles fixed. May be useful with cryostats or other equipment which cannot rotate much. Obviously, *s1*, *s2*, and *s3* must all be different.
- `setmode` *d1 a1 s1* *s1* can be any sample circle, or the special values 5 or 6 for eta=del/2 or mu=nu/2 respectively
- `setmode 0` *a1 s1 s2* selects one azimuthal and two sample constraints. Allegedly, the mu-fixed plus phi-fixed mode isn't working.
- `setmode` *d1* `0` *s1 s2* selects one detector and two sample constraints. Allegedly, the eta-fixed plus phi-fixed, eta-fixed plus chi-fixed, and naz-fixed modes aren't working.

3.2.2 Azimuth

In psic, selection of the azimuth can be done with angles as well as with Miller indices. To specify by angles, the commmand is
`setaz` *sigma tau*
where *sigma* and *tau* are the chi and phi angles. To specify by Miller indices, the command is
`setaz` $h\ k\ \ell$
The macro sigtau tells how to specify the azimuth:
`sigtau 1`
is for selection by angles, and
`sigtau 0`
is for selection by Miller indices.

If you are working with a sample whose surface normal is the azimuth, then it's convenient to use the `setaz2` macro. First, find (or know) the values of phi and chi that make the surface normal parallel to the eta axis; this is often done by reflecting a laser beam, if the surface is reflective. (Specifically, adjust phi and chi until the reflected beam does not move when eta is rotated). These values are called flat_phi and flat_chi, and are like tau and sigma except for a sign (or signs). Then, at the SPEC command line, type
`setaz2`
and you can use the current angular positions or enter your own.

3.2.3 Sectors and cut points

In psic geometry, the additional motors lead to additional sector transformations, 16 in all. They are listed in SPEC's psic help file. In psic, use the command
`sector` *value*
(not `setsector`, as in kappa geometry) to choose which transformation to use (if you leave off *value*, you will be prompted for it). You could also set the variable g_sect to the number of the transformation you wish:
`g_prefer =` *value*.

Fortunately, there is a handy alternative in psic to keeping track of all the angular positions in the 16 different sectors. Sector 0, instead of selecting a certain transformation, ranks all the transformations according to convenience. The ranking schemes are chosen by the variable `g_prefer`, but so far, only two have been implemented: `g_prefer = 1` is for a 'vertical' diffractometer ($0 \leq$ del <180 and $-90 \leq$ nu ≤ 90), which is the appropriate choice for the Newport kappa diffractometer in 7-ID-C. `g_prefer = 2` is for a 'horizontal' diffractometer ($-90 \leq$ del <90 and $0 \leq$ nu <180). One could still use the `sectors` command, as described in Section 3.1.3.

Cut points in psic operate as they do in kappa, so see Sec. 3.1.3 for full details. The difference is that psic has nine cut points instead of seven, due to the addition of the nu and mu motors. Again, cut points of -180 are ususally fine as default values, but eta and keta operate a bit smoother with cut points of -170.

3.3 Scanning (and miscellaneous) hints

Since a chi scan actually moves three real motors, some users of Newport kappas have experienced problems with motions in theta during a chi scan. (The real motor, k-theta, does of course move during a chi scan, just not as precisely as sometimes needed.) Therefore, instead of performing chi scans like
`dscan chi -1 1 20 1`
some users have made the recommendation to explicitly tell SPEC that theta (or eta) should be

fixed:

```
d2scan chi -1 1 th 0 0 20 1
```

This might be less of a problem with trajectory scanning than point-by-point scanning (see Sec. 6).

Reciprocal-space scans should be done carefully. Because of the limited resolution of the servo motors, a `ubr`-type command may not be sufficiently close to its intended position. For instance, consider the two commands

```
ubr 1 0 0.1
lscan 0.1 1.9 18 1
```

The user is obviously intending to scan from $\ell = 0.1$ to 1.9 at $h = 1$ and $k = 0$. However, depending on the "retry deadband" of the servo motors (i.e., the effective angular resolution), the diffractometer may end up at $h = 0.9994$ and $k = 0.00013$, as an example. The `lscan` that follows will be performed at $h = 0.9994$ and $k = 0.00013$, *not* at $h = 1$ and $k = 0$ as intended. Thus, the desired values of h and k should be entered explicitly:

```
hklscan 1 1 0 0 0.1 1.9 18 1
```

This command forces h and k to their intended values, rather than hoping their current values are close enough.

The distance from the top of the X95 rail carrier on the delta arm to the $x = 0$ plane (see Fig. 1) is 281 mm. This distance will be important when designing a detector mount.

Note that power to the motors on the MM4005 should be on before complex motor motions are made, e.g., moving chi or to a certain reciprocal lattice point. The problem is that some motors may receive the command to move before they have power, and therefore will not move. Keep this in mind after tripping a limit switch or hitting the red Emergency Stop button.

4 Linear Motions

There are three linear sample motions, plus five to move the whole diffractometer. The sample motions are samplex, sampley, and samplez, with z along the phi axis. These are not high-precision motors, designed only for moving the sample to the center of rotation and not for fine scanning. Furthermore, they may have backlash issues which need to be dealt with. The base of the diffractometer has five motors, so it is not quite kinematical. Three vertical jacks are labeled Y1, Y2, and Y3. Xtranslation moves the diffractometer horizontally, transverse to the beam. And AY is a rotation about a vertical axis (specifically, it pivots about the Y2 motor).

4.1 Table pseudomotors

Tom Trainor of CARS has developed an EPICS table record to convert from these real motors to rotations about the diffractometer's center of rotation. This table record also allows the diffractometer to be moved and rotated for an x-ray beam deflected by Kirkpatrick-Baez (KB) mirrors. Eight pseudomotors, listed in Table 5, effectively move the table about its center, D0. Two EPICS screens are shown in Fig. 4; in the left screen, you enter the distance from D0 to the mirrors (the other distances should be correct), and the screen on the right defines the lengths and directions. The following procedure describes how to use the table pseudomotors to quickly align the diffractometer with KB mirrors. It uses the right-hand rule:

- First, get the direct beam thru D0. Follow the traditional steps of locating D0 (the center of rotation) with a pin or other small object, getting the beam on the pin, and then taking burns in front and back to make sure the incident beam is square to the diffractometer (i.e, perpendicular to the del/eta and mu/nu axes).
- It's a good idea to adjust the EPICS offsets of the real motors to be zero. This is not necessary but can help avoid unintended movements later.
- Check that you entered the distances from D0 to the mirrors on the newport_table_calcs.adl EPICS screen.
- Rotate the diffractometer about D0 by the angles at which the beam is deflected: Move AY by twotheta of the horizontal mirror and AX by negative twotheta of the vertical mirror. (This assumes the typical KB geometry of deflecting upward and outboard.)
- If the KB mirrors are mounted on the kappa's input pillar, then they have rotated too; they must both be rotated by negative twotheta (note the kludge in the way positive rotation is defined).
- Translate the diffractometer such that D0 is now on the deflected ray: Move R_AY by twotheta of the horizontal mirror and R_AX by negative twotheta of the vertical mirror.
- Check that the beam is still on D0. Since it's difficult to know the exact twotheta of the KB mirrors (angular motion per motor step is not constant for the mirrors' rotations), it is better to tweak the mirror angle than to move the diffractometer all around.

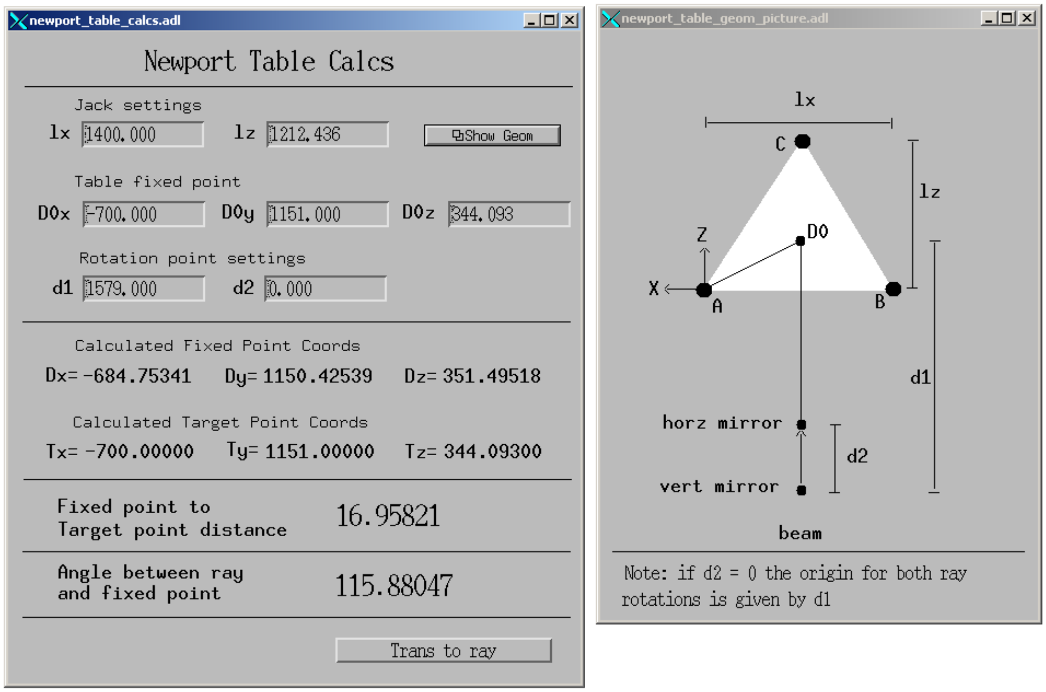

Figure 4: EPICS screens to use the CARS table motor record. Values are entered in the left screen; the "Show Geom" button of the left screen brings up the screen on the right. The "Translate to ray" button seems to force the pseudomotors to be updated; hit it if the pseudomotor screens don't make real motors move, but don't hit it if you don't want motors to move!

Pseudomotor	Description
AX	Rotate diffractometer at D0 about X axis.
AY	Rotate diffractometer at D0 about Y axis.
AZ	Rotate diffractometer at D0 about Z axis.
R_X	Translates ray in X direction (and translates D0 to ray)
R_Y	Translates ray in Y direction (and translates D0 to ray)
R_Z	Basically just adjusts the focal length
R_AX	Rotates ray about X axis (and translates D0 to ray)
R_AY	Rotates ray about Y axis (and translates D0 to ray)

Table 5: List of pseudomotors for moving the diffractometer table. D0 is the center of rotation; the right-hand rule applies.

5 Homing Motors and Hardware Limits

It's often a good idea to home the diffractometer's motors before use. Do this on the MM4005 front panel, or in the "debug" motor screen of EPICS. Table 6 presents the home positions; it is often practical to move a motor close to its home position before hitting the home switch. Also shown are the maximum "dial limits" as stored in the MM4005 controller. Convert to EPICS or SPEC user units via the offset and direction, which are stored in EPICS. To avoid collisions, tighter limits are often set in EPICS. The limits entered in the MM4005 may also be tighter when a collision danger is always present [e.g., tth above 160° in user units (below 20° in dial units) will probably crash the detector arm into the incident-beam flight path].

Motor Name(s)	MM4005 dial values			EPICS values	
	Home	Neg. Limit	Pos. Limit	Direction	Offset
Top MM4005 controller: Diffractometer angles					
phi/kphi	0	-183	185	neg	0 (arbitrary)
kappa	0.6402	-182	189	neg	0
omega/kth/keta	89.8325	-180	360	neg	180
psi/mu	3.88	-193	61	neg	1.83
2-theta/tth/del	89.719	-12	190	neg	180*
nu	0.04175	-61	194	neg	0
Bottom MM4005 controller: Table motors and sample stages					
Y1	0†	-115	60	pos	3.5‡
Y2	0†	-115	60	pos	3.5‡
Y3	0†	-115	60	pos	3.5‡
RotAY	0	-24	24	pos	-10‡
Xtrans	0	-57	46	neg	1.07‡
samplex	0	-3	3	pos	0
sampley	0	-2.8	2.7	pos	0
samplez	0**	0	30	pos	0

Table 6: Home and limit positions for motors on the kappa diffractometer. Note that MM4005 values are in dial units; user = (dir)*dial + offset; thus *be careful* and note that dial directions are in most cases opposite of user directions! The limits are the maximum ranges; the software limits in EPICS are typically tighter.
Key:
* This offset can be adjusted based on how your detector (or slits) are mounted.
†Home positions of Y1, Y2, and Y3 are at a gap of approx. 116 mm in the housing near each jack.
‡Offsets of table motors must be adjusted such that the direct (nondeflected) beam passes through the center of rotation when these motors are at zero (in user units). Otherwise, the table pseudo-motors will not operate correctly.
** Home position of samplez is at bottom of travel.

6 Trajectory Scanning

Using a procedure developed at GSE-CARS, trajectory scanning is available when operating the kappa with SPEC. Instead of point-by-point scans performed by moving to a point, stopping, and counting (repeating ad nauseum), trajectory scans move motors continuously, with the counts being binned along the way and read out at the end. Such scans can greatly reduce the overhead time in making a scan. Most of the normal SPEC scans can be performed since the trajectories are nonlinear and can handle moving all motors. The SPEC shortcut macro to turn on trajectory scanning is `ton`, and to return to point-by-point scannning (the default) is `toff`.

Trajectory scans take into account the acceleration and deceleration of the servo motors, so even in the simplest `ascan`, motor speed is not continuous. That means there are usually more counts in the first few and last few points of a scan, since the motors are moving slower. Thus, to avoid confusion one must normalize the counts, if not to a stable ion chamber, then at least to the count time. A macro named `sc_an` normalizes the most recent scan to count time, and calculates some statistics like peak position and FWHM. Trajectory scanning works best with real-motor scans, since the trajectory is so much easier to calculate; particularly complex scans (such as reciprocal-space scans) may not work well in trajectory mode if the motors have a hard time following the calculated trajectory. The listed motor (or reciprocal-space) positions in a trajectory scan are by default the actual values, so you can tell how accurate a given scan was (although you can show the ideal positions if you wish).

The scaler board which must be used in trajectory scanning is manufactured by Struck (aka SIS); it receives pulses from the MM4000 indicating when to bin the counts and is currently configured for eight counters. Checks are made to ensure the diffractometer doesn't move much too fast or too slow, but still be careful to scan with reasonable motor velocities. A strange bug in the Struck board, when used as the timer, is that when you tell it to count for t seconds, it seems to always count for $t + 0.01$ sec.

Note that time for the Struck is usually kept with the 1-MHz clock of a V-to-F NIM unit, rather than the 10-MHz clock of the Joerger scaler (to avoid overflow). If you switch boards in SPEC, then be sure to update the clock speed in the counters menu of config. Many of the trajectory-scanning SPEC macros from GSE-CARS assume that the "monitor" `MON` is the timebase, not a detector like an ion chamber.

Error messages are returned if you try to perform an illegal scan, e.g., one that moves the motors too fast. However, sometimes error messages just happen; this often occurs the first time you do a trajectory scan. If you repeat the same scan, it will often be able to be performed. Try to avoid canceling a trajectory scan, especially in the trajectory-building stage, with a CTRL-C.

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