```
PRINTER LOGFILE at Tue Jul 16 12:23:54 2013 from opid20
Current Positions  (user, dial)
  TTH hor        SRZ        SRX        SRY       ASLH       ASLV
      tth         th        chi        phi       aslh       aslv
 19.078925   0.000000   0.000000   0.000000   0.000000   0.000000
 19.321900   0.243250   0.000000   0.000000   0.000000   0.000000

      KBX        KBY      KBT3Z      KBR3Y     KBROTY        pi3
      kbx        kby      kbt3z      kbr3y     kbroty        pi3
-39.999900   3.396300   0.732094   0.669119   3.174792   0.000000
-39.999900   3.396300   0.732094   0.669119   3.174792   0.000000

      KBZ      KBBU3      KBBD3      KBR4Z     KBRT4Z        pi4
      kbz      kbbu3      kbbd3      kbr4z     kbrt4z        pi4
 0.354267 11160.00000 -1726.00000   6.078003   0.692901   0.000000
 0.354267 11160.00000 -1726.00000   6.078003   0.692901   0.000000

    KBBDU4      KBBD4     i1vgap      i1vof     i1hgap     i1hof
    kbbu4      kbbd4     i1vgap      i1vof     i1hgap     i1hof
1210.000000 -1650.00000   1.000000  -2.725516   1.000000   2.325535
1210.000000 -1650.00000   1.000000  -2.725516   1.000000   2.325535

      STZ        STY        STX       SRTX       SRTY        ax1
      stz        sty        stx       srtx       srty        ax1
 0.000000   0.000000   0.000000   0.000000   0.000000 1976.444500
 0.000000   0.000000   0.000000  -0.052550   0.218650 1976.444500

      az1       ath1      achi1     achim1        ax2        az2
      az1       ath1      achi1     achim1        ax2        az2
21.753000  86.187606   0.054120   0.047204 1984.447000   5.454000
21.753500  80.566968   0.054120  -1.655230 1984.447000   5.454000

     ath2      achi2     achim2        ax3        az3       ath3
     ath2      achi2     achim2        ax3        az3       ath3
85.716277   0.027202   0.023726 1974.591500   0.000000  85.559415
79.801968   0.027202  -0.900815 1974.591500   0.000000  78.952181

    achi3     achim3        ax4        az4       ath4      achi4
    achi3     achim3        ax4        az4       ath4      achi4
 0.000000   0.000000 1980.502000   5.443000  85.716277  -0.027213
 0.000000  -0.129171 1980.502500   5.443000  80.350000  -0.027213

   achim4        ax5        az5       ath5      achi5     achim5
   achim4        ax5        az5       ath5      achi5     achim5
-0.023727 1978.417000  21.774500  86.187606  -0.054132  -0.047193
 1.077609 1978.417500  21.774500  80.044734  -0.054132   0.774530

  TTH ver Detector x Detector z   Det. Rot.    TABLE y      hrtx5
     tthv        dtx        dtz       drot         ty      hrtx5
 0.539475 -113.832800 287.353755 171.118850   1.076683   3.325079
 0.539475  -88.206700 205.328375 170.992750   1.076683   3.325079

    hrth5     hrchi5  Anal Bragg Anal Energy  APD 11th MAXIPIX thl
    hrth5     hrchi5        ath    energy2       11th     mpxthl
-0.809822  -0.100000  85.559415  11.217500   1.037500 6825.000000
-0.809822  -0.100000  85.559415  11.217500   1.037500 6825.000000

   energy   Motor 69   beamstop   APD2 11th       p3th       p3wl
   energy        m69      bstop      11th2       p3th       p3wl
11.217500   0.000000  -9.000000   1.966000  85.601996   0.055245
11.217500   0.000000  -9.000000   1.966000  -3.857154   0.055245
```

```
   mbvss1     LS336A     LS336B     LS336C     LS336D    euro422
   mbvss1      1336A      1336B      1336C      1336D    euro422
 0.000000 295.000000   0.000000   0.000000   0.000000 580.000000
 0.000000 295.000000   0.000000   0.000000   0.000000 580.000000

Four-Circle Geometry, Phi fixed (Three-circle) (mode 3)
Sector 0

   Primary Reflection (at lambda 1.10488):
        tth th chi phi = 83.5491 31.4582 -1.023 0
            H K L = 0 0 16

   Secondary Reflection (at lambda 1.10488):
        tth th chi phi = 84.7203 40.2811 -1.096 0
            H K L = 0.5 0.5 16

   Lattice Constants (lengths / angles):
          real space = 4.03 4.03 13.28 / 90 90 90
      reciprocal space = 1.559 1.559 0.473 / 90 90 90

   Azimuthal Reference:
            H K L = 0 0 1

            Lambda = 1.10488

Cut Points:
     tth   th  chi  phi
    -180 -180 -180 -180
```

ID20 experimental form

Dates: 17 - 23.07.2013

	Shifts:
☐ Non-resonant	
☒ Resonant	18

Data directory: run3-13 / run7-hc738

Title:

Code: HC 738

Main proposer: K. OHGUSHI

Users:

LC: M. MORETTI

Ring filling mode, max. current: 200 mA

Optical elements:

Undulators and harmonics: 4 × U26

Spectrometer: RIXS (2m)

Beam size on sample:

Energy range: ~11.215 keV

Detectors + SCA limits:

Analysers: 5 × Si (844) diced

Monitors:

Other observations:

batch 1 Δ

#2   stz = - 5.56

#3   stz = - 4.228

#4   stz = - 2.478

#5   stz = - 0.545

#1   stz = - 7.996

th set from -2.176 to 0   for sample #2

sample #2 ; one reflection / x ui plane

th = 36.548 ; chi = -3

sec./ th = 26.497 ; chi = +1

#3 ; (i)   th = 28.392 ; chi = 0

(ii) th = 38.364 ; chi = 0 -4

Refine #3 ; (ii)

Jul 17, 13 12:14 — **ppopid20fourc.log** — Page 1/1

```
PRINTER LOGFILE at Wed Jul 17 12:14:57 2013 from opid20
                STZ         STY         STZ
                stz         sty         stz
User
 High       22.000000   20.000000   22.000000
 Current    -2.441644    0.355150   -2.441644
 Low       -22.000000  -20.000000  -22.000000
Dial
 High       22.000000   20.000000   22.000000
 Current    -2.441644    0.355150   -2.441644
 Low       -22.000000  -20.000000  -22.000000

                TTH hor     SRZ         SRX         SRY
                tth         th          chi         phi
User
 High      110.02702   181.93260    10.00000     7.00000
 Current    81.40250    38.34708    -4.13200     0.00000
 Low        -4.97298   -88.06740   -10.00000    -7.00000
Dial
 High      110.27000   180.00000    10.00000     7.00000
 Current    81.64548    36.41448    -4.13200     0.00000
 Low        -4.73000   -90.00000   -10.00000    -7.00000
```

th real = 76.1525

→ 5.25

(008) ?

Jul 17, 13 12:33 — **ppopid20fourc.log** — Page 1/1

```
PRINTER LOGFILE at Wed Jul 17 12:33:25 2013 from opid20
                STZ         STY         STZ
                stz         sty         stz
User
 High       22.000000   20.000000   22.000000
 Current    -2.441644    0.355150   -2.441644
 Low       -22.000000  -20.000000  -22.000000
Dial
 High       22.000000   20.000000   22.000000
 Current    -2.441644    0.355150   -2.441644
 Low       -22.000000  -20.000000  -22.000000

                TTH hor     SRZ         SRX         SRY
                tth         th          chi         phi
User
 High      110.02702   181.93260    10.00000     7.00000
 Current    55.95000    28.34510    -1.40000     0.00000
 Low        -4.97298   -88.06740   -10.00000    -7.00000
Dial
 High      110.27000   180.00000    10.00000     7.00000
 Current    56.19297    26.41250    -1.40000     0.00000
 Low        -4.73000   -90.00000   -10.00000    -7.00000
```

(0 0 6) ?

set as 0r0

56.00

Jul 17, 13 13:54 — **ppopid20fourc.log** — Page 1/1

```
PRINTER LOGFILE at Wed Jul 17 13:54:09 2013 from opid20
                STZ         STY         STZ
                stz         sty         stz
User
 High       22.000000   20.000000   22.000000
 Current    -2.463208    0.355000   -2.463208
 Low       -22.000000  -20.000000  -22.000000
Dial
 High       22.000000   20.000000   22.000000
 Current    -2.463208    0.355000   -2.463208
 Low       -22.000000  -20.000000  -22.000000

                TTH hor     SRZ         SRX         SRY
                tth         th          chi         phi
User
 High      110.02702   181.93260    10.00000     7.00000
 Current    55.95842    28.30660    -1.28800    -1.28600
 Low        -4.97298   -88.06740   -10.00000    -7.00000
Dial
 High      110.27000   180.00000    10.00000     7.00000
 Current    56.20140    26.37400    -1.28800    -1.28600
 Low        -4.73000   -90.00000   -10.00000    -7.00000
```

(206)

(026) !
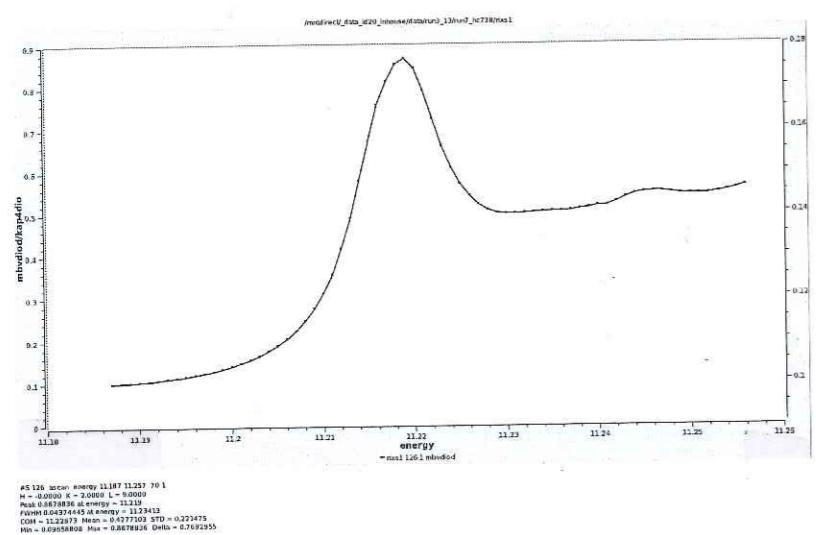
Jul 17, 13 14:11 — **ppopid20fourc.log** — Page 1/1

```
PRINTER LOGFILE at Wed Jul 17 14:11:04 2013 from opid20
                STX         STY         STZ
                stx         sty         stz
User
 High       20.000000   20.000000   22.000000
 Current     0.000000    0.355000   -2.452040
 Low       -20.000000  -20.000000  -22.000000
Dial
 High       20.000000   20.000000   22.000000
 Current     0.000000    0.355000   -2.452040
 Low       -20.000000  -20.000000  -22.000000

                TTH hor     SRZ         SRX         SRY
                tth         th          chi         phi
User
 High      110.02702   181.93260    10.00000     7.00000
 Current    76.15250    38.35040    -4.50000    -1.28600
 Low        -4.97298   -88.06740   -10.00000    -7.00000
Dial
 High      110.27000   180.00000    10.00000     7.00000
 Current    76.39548    36.41780    -4.50000    -1.28600
 Low        -4.73000   -90.00000   -10.00000    -7.00000
```

(028) !
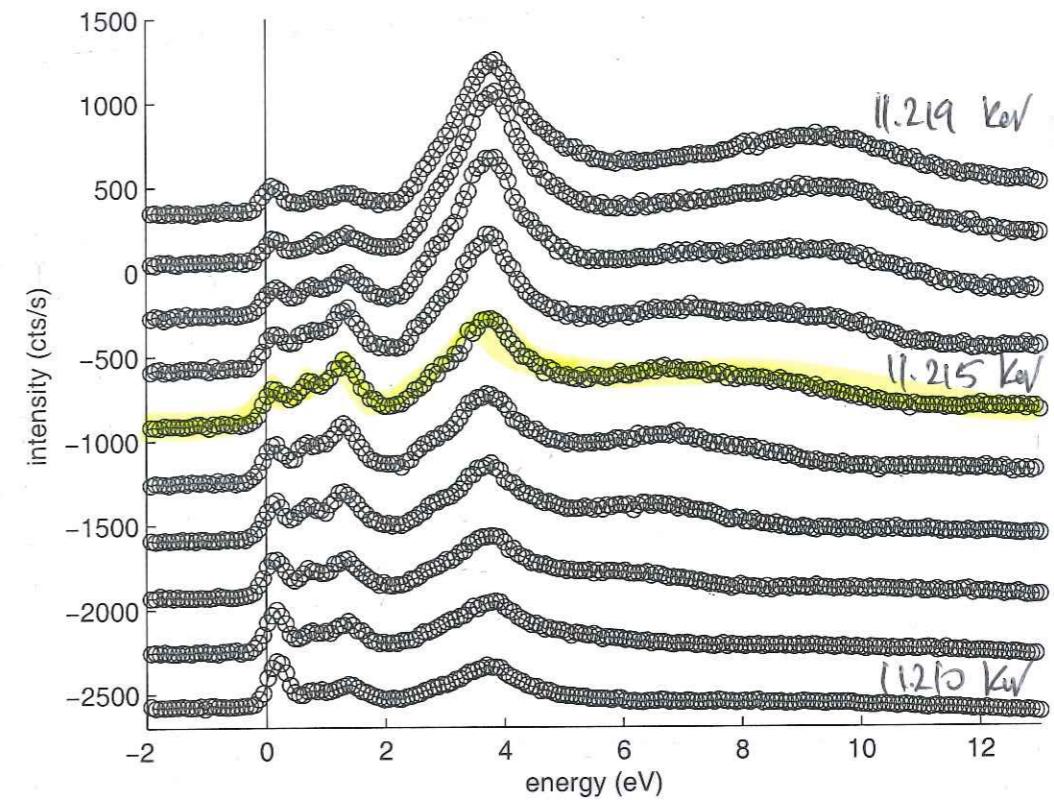
Scan # 12C

#197   ubr (0,2,9)   ascan energy 2   A[energy]+0.003
                                        A[energy]-0.013



```
 Jul 17, 13 18:25          ppopid20fourc.log           Page 1/1
PRINTER LOGFILE at Wed Jul 17 18:25:01 2013 from opid20
# /mntdirect/_data_id20_inhouse/data/run3_13/run7_hc738/CaIrO3.mac
def lowRes '{

shopen
ccdon
plotselect roi3

local EEEEE

  for (EEEEE=11.219;EEEEE>11.208;EEEEE-=.001) {

   p EEEEE
   umv energy EEEEE                              #204
   ascan energy2 A[energy]+0.002 A[energy]-0.013 200 4

  }
}'
```

#204	11.219
#205	11.218
#206	
#213	11.210

Choose   Emc = 11.215 keV

We stick to Em = 11.215 keV, which we found to maximize the low energy features. We move to high-energy-resolution Si(844) IN - Si(311) OUT

#237 elastic line on scotch tape $\Delta E_3 \cong 25$ meV

Align the sample @ room temperature

```
Jul 18, 13 4:23                    ppopid20fourc.log                    Page 1/1

PRINTER LOGFILE at Thu Jul 18 04:23:25 2013 from opid20
# /mntdirect/_data_id20_inhouse/data/run3_13/run7_hc738/CaIrO3.mac
def firstnight '{
                          T-258 K
shopen
ccdon
plotselect roi3

ubr 0 2 9
umv stx 0.2516 sty -0.06880 stz 3.03514            #342
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 0 2 9.5
umv stx 0.2442 sty -0.06880 stz 3.06774            #343
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 0 2 10
umv stx 0.237 sty -0.06880 stz 3.07013             #344
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 1 2 9
umv stx 0.44420 sty -0.06880 stz 3.0749            #345
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr .5 2 9
umv stx 0.2851 sty -0.06880 stz 3.07546
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

}'
```

```
Jul 18, 13 18:44                   ppopid20fourc.log                    Page 1/1

PRINTER LOGFILE at Thu Jul 18 18:44:34 2013 from opid20
              SRZ        TTH hor       SRX         SRY
               th          tth         chi         phi
User
  High      179.93260   110.02702    10.00000     7.00000
  Current    50.25430   100.18953     4.13800     0.00000
  Low       -90.06740    -4.97298   -10.00000    -7.00000
Dial
  High      180.00000   110.27000    10.00000     7.00000
  Current    50.32170   100.43250     4.13800     0.00000
  Low       -90.00000    -4.73000   -10.00000    -7.00000

              STX         STY         STZ
              stx         sty         stz
User
  High      20.000000   20.000000   22.000000
  Current    0.131000   -1.109000    3.043000
  Low      -20.000000  -20.000000  -22.000000
Dial
  High      20.000000   20.000000   22.000000
  Current    0.131000   -1.109000    3.043000
  Low      -20.000000  -20.000000  -22.000000

Four-Circle Geometry, Phi fixed (Three-circle) (mode 3)
Sector 0

  Primary Reflection (at lambda 1.10488):
          tth th chi phi = 100.19 50.2543 4.138 0
                 H K L = 0 2 10

  Secondary Reflection (at lambda 1.10488):
          tth th chi phi = 90.6857 15.8134 2.225 0
                 H K L = 2 2 8

  Lattice Constants (lengths / angles):
          real space = 3.147 9.859 7.29 / 90 90 90
     reciprocal space = 1.997 0.6373 0.8619 / 90 90 90

  Azimuthal Reference:
                 H K L = 0 0 1

              Lambda = 1.10488

Cut Points:
       tth    th   chi  phi
      -180  -180  -180  -180
```

0v0

0 2 10

```
Jul 18, 13 16:05                   ppopid20fourc.log                    Page 1/1

PRINTER LOGFILE at Thu Jul 18 16:05:59 2013 from opid20
              SRZ        TTH hor       SRX         SRY
               th          tth         chi         phi
User
  High      179.93260   110.02702    10.00000     7.00000
  Current    38.24428    76.30575     2.22050     0.00000
  Low       -90.06740    -4.97298   -10.00000    -7.00000
Dial
  High      180.00000   110.27000    10.00000     7.00000
  Current    38.31168    76.54873     2.22050     0.00000
  Low       -90.00000    -4.73000   -10.00000    -7.00000

              STX         STY         STZ
              stx         sty         stz
User
  High      20.000000   20.000000   22.000000
  Current    0.213100   -1.129200    3.039022
  Low      -20.000000  -20.000000  -22.000000
Dial
  High      20.000000   20.000000   22.000000
  Current    0.213100   -1.129200    3.039022
  Low      -20.000000  -20.000000  -22.000000
```

0r1

(0 2 8)

```
Jul 18, 13 18:34                   ppopid20fourc.log                    Page 1/1

PRINTER LOGFILE at Thu Jul 18 18:34:56 2013 from opid20
              SRZ        TTH hor       SRX         SRY
               th          tth         chi         phi
User
  High      179.93260   110.02702    10.00000     7.00000
  Current    15.81338    90.68573     2.22500     0.00000
  Low       -90.06740    -4.97298   -10.00000    -7.00000
Dial
  High      180.00000   110.27000    10.00000     7.00000
  Current    15.88077    90.92870     2.22500     0.00000
  Low       -90.00000    -4.73000   -10.00000    -7.00000

              STX         STY         STZ
              stx         sty         stz
User
  High      20.000000   20.000000   22.000000
  Current    0.535000   -1.109000    3.053522
  Low      -20.000000  -20.000000  -22.000000
Dial
  High      20.000000   20.000000   22.000000
  Current    0.535000   -1.109000    3.053522
  Low      -20.000000  -20.000000  -22.000000
```
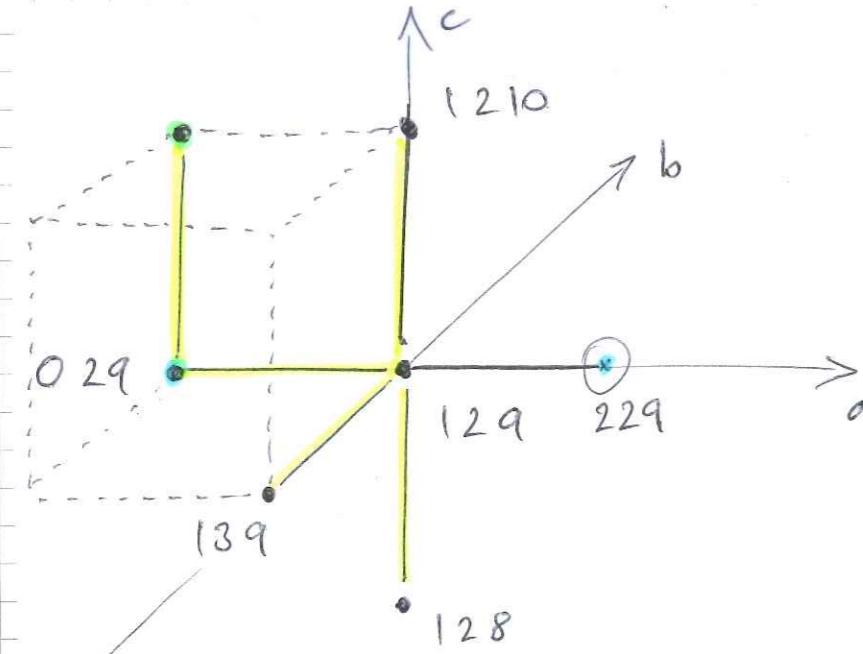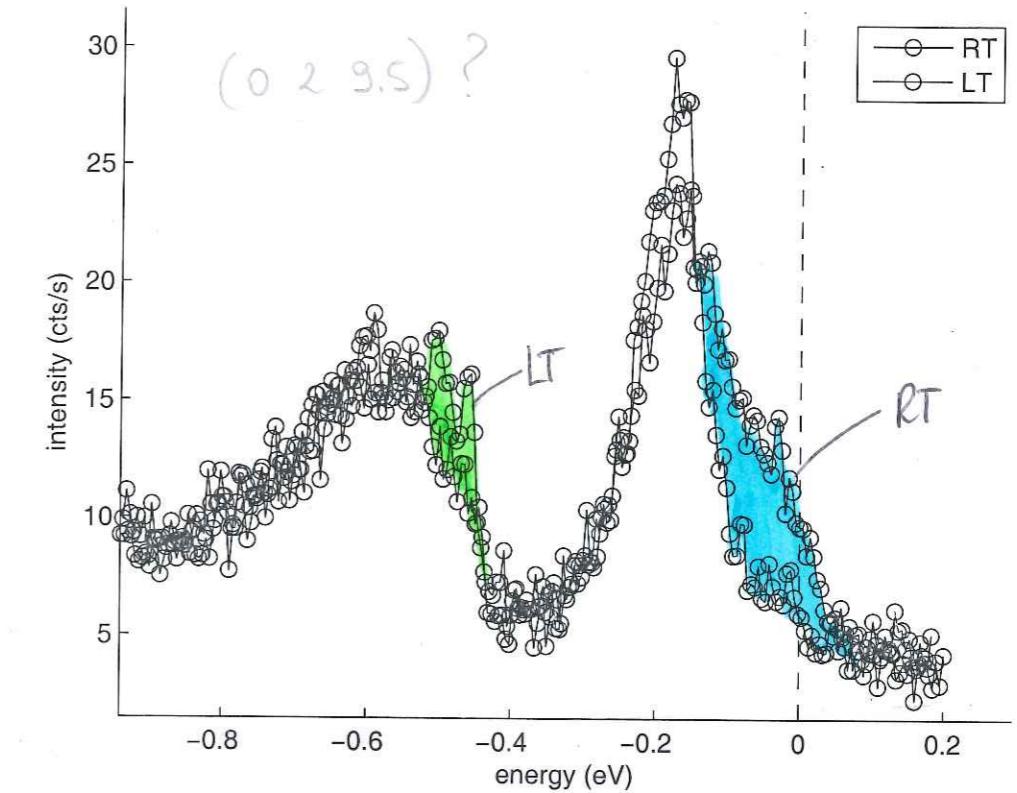
0r1

2 2 8

```
Jul 18, 13 23:48              ppopid20fourc.log                Page 1/2
PRINTER LOGFILE at Thu Jul 18 23:48:44 2013 from opid20
# /mntdirect/_data_id20_inhouse/data/run3_13/run7_hc738/CaIrO3.mac
def secondnight '{

shopen
ccdon
plotselect roi3

#ubr 0 2 9
#umv stx 0.22445 sty -1.10900 stz 3.05763
#ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 0 2 9.2
umv stx 0.225150 sty -1.10900 stz 3.058660
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 0 2 9.4
umv stx 0.2114 sty -1.10900 stz 3.06062
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 0 2 9.5
umv stx 0.19995 sty -1.10900 stz 3.06166
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 0 2 9.6
umv stx 0.2037 sty -1.10900 stz 3.06062
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 0 2 9.8
umv stx 0.18905 sty -1.10900 stz 3.07017
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 0 2 10
umv stx 0.166 sty -1.10900 stz 3.07503
ascan energy2 A[energy]+-.0002 A[energy]-0.0018 320 10

ubr 0.2 2 9.8
umv stx 0.21585 sty -1.10900 stz 3.06424
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10

ubr 0.4 2 9.6
umv stx 0.24855 sty -1.10900 stz 3.05728
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```

T = 30 K

#543
#546
#547
#548
#549
#550
551
552
553

$$\text{In[10]:= } \text{Chop}\left[\text{NSolve}\left[\left\{\frac{\sqrt{3}}{2}\sqrt{3\,\xi^2 + 4\,\xi\,\Delta + 12\,\Delta^2} == 1.3, \frac{3}{4}\xi - \frac{3}{2}\Delta + \frac{\sqrt{3}}{4}\sqrt{3\,\xi^2 + 4\,\xi\,\Delta + 12\,\Delta^2} == .6\right\}, \{\xi, \Delta\}\right]\right]$$

$$\text{Out[10]= } \{\{\xi \to -0.563532, \Delta \to -0.248433\}, \{\xi \to 0.496866, \Delta \to 0.281766\}\}$$

estimate of ξ & Δ

$$\text{In[28]:= } A = \frac{-\xi - 6\,\Delta + \sqrt{3}\sqrt{3\,\xi^2 + 4\,\xi\,\Delta + 12\,\Delta^2}}{2\,\xi} \;/.\; \xi \to 0.497 \;/.\; \Delta \to 0.282$$

$$\text{Out[29]= } 0.414988$$

$$\text{In[34]:= } \text{MAG} = \frac{(A-1)^4}{(A^2 - 2A - 2)^2}$$

$\frac{I_{L_2}}{I_{L_3}}$ RXMS

$$\text{ATS} = \frac{1}{4}\frac{(A-1)^4}{(A^2 + A - 2)^2}$$

ATS

$$\text{Out[34]= } 0.0165816$$

$$\text{Out[35]= } 0.0146703$$

$$\text{In[35]:= } \frac{1}{\sqrt{A^2 + 2}}\{A, 0, 0, 1, 0, i\}$$

admixture of states in $\{xy+, xy-, yz+, yz-, zx+, zx-\}$

$$\text{Out[36]= } \{0.281569, 0., 0., 0.678498, 0., 0. + 0.678498\, i\}$$

(0 2 9.5) ?

```
Jul 19, 13 12:02          ppopid20fourc.log          Page 1/2

PRINTER LOGFILE at Fri Jul 19 12:02:14 2013 from opid20
# /mntdirect/_data_id20_inhouse/data/run3_13/run7_hc738/CaIrO3.mac
def thirdday '{

shopen
ccdon
plotselect roi3

ubr 0.5 2 9.5
umv stx 0.2584 sty -1.10900 stz 3.06063
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #554

ubr 0.6 2 9.4
umv stx 0.2307 sty -1.10900 stz 3.05558
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #555

ubr 0.7 2 9.3
umv stx 0.255 sty -1.10900 stz 3.052
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #556

ubr 0.8 2 9.2
umv stx 0.2822 sty -1.10900 stz 3.04964
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #557

ubr 0.9 2 9.1
umv stx 0.285 sty -1.10900 stz 3.044
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #558

ubr 1 2 9
umv stx 0.29165 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #559

ubr 0.9 2 9
umv stx 0.28 sty -1.10900 stz 3.049
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #560

ubr 0.8 2 9
umv stx 0.27245 sty -1.10900 stz 3.04977
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #561

ubr 0.7 2 9
umv stx 0.269 sty -1.10900 stz 3.04982
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #562

ubr 0.6 2 9
umv stx 0.2667 sty -1.10900 stz 3.04982
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #563

ubr 0.5 2 9
umv stx 0.25685 sty -1.10900 stz 3.044
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #564

ubr 0.4 2 9
umv stx 0.24685 sty -1.10900 stz 3.05741
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #565

ubr 0.3 2 9
umv stx 0.244 sty -1.10900 stz 3.05827
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #566

ubr 0.2 2 9
umv stx 0.2427 sty -1.10900 stz 3.05827
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10    #567
```
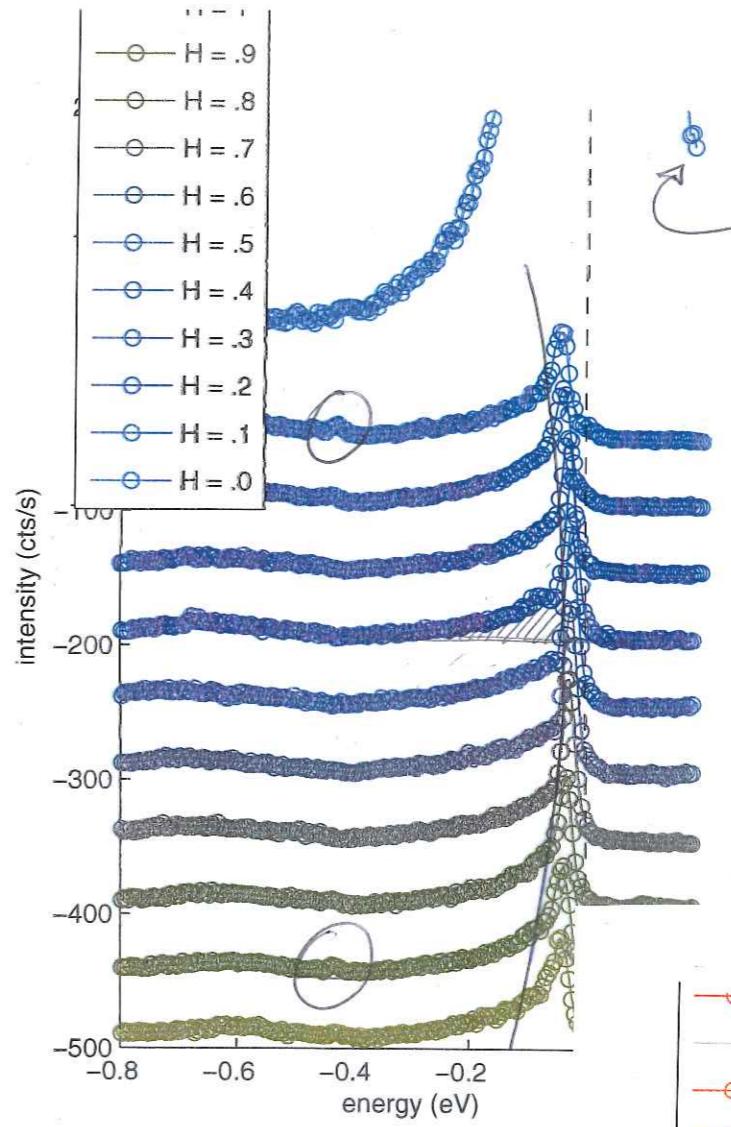
?
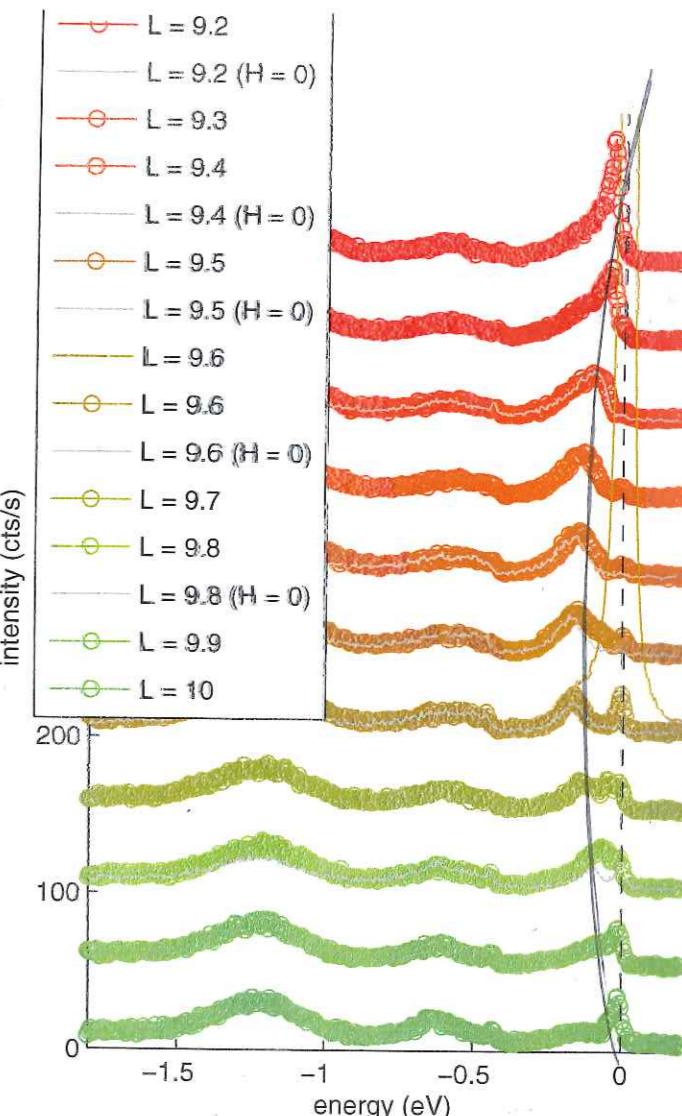
Recalibrate the incident energy on a magnetic Bragg peak

#599 before resetting of p3th & rmth
#601 after resetting

(H, 2, 9) dispersion

— (0, 2, 9) magnetic Bragg peak

gapped mode with tiny (~15 meV) dispersion along (a)

multiple magnetic excitation?

(1, 2, L) dispersion

CaIrO3.mac

2013-07-20

```
ubr 0.1 2 9
umv stx 0.23 sty -1.10900 stz 3.05763
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#606

```
ubr 0 2 9
umv stx 0.22445 sty -1.10900 stz 3.05763
ascan energy2 A[energy]+.0002 A[energy]-0.002 80 2
```
#607

```
ubr 1 2 9
umv stx 0.29165 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 2
```
#608

```
ubr 1 2 9.1
umv stx 0.32825 sty -1.10900 stz 3.06212
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#609

```
ubr 1 2 9.2
umv stx 0.2784 sty -1.10900 stz 3.06291
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#610

```
ubr 1 2 9.3
umv stx 0.2794 sty -1.10900 stz 3.06391
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#611

```
ubr 1 2 9.4
umv stx 0.27985 sty -1.10900 stz 3.06466
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#612

```
ubr 1 2 9.5
umv stx 0.27885 sty -1.10900 stz 3.06466
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#613

```
ubr 1 2 9.6
umv stx 0.27735 sty -1.10900 stz 3.06827
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#614

2013-07-20

```
ubr 1 2 9.6
umv stx 0.47735 sty -1.10900 stz 3.06827
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#619

```
ubr 1 2 9.7
umv stx -0.0535 sty -1.10900 stz 3.05917
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#620

```
ubr 1 2 9.8
umv stx 0.2716 sty -1.10900 stz 3.07113
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#621

```
ubr 1 2 9.9
umv stx 0.307 sty -1.10900 stz 3.06917
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#622

```
ubr 1 2 10
umv stx 0.257 sty -1.10900 stz 3.07276
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#623

```
ubr 0.9 2 9.9
umv stx 0.26405 sty -1.10900 stz 3.07095
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#624

```
ubr 0.8 2 9.8
umv stx 0.25625 sty -1.10900 stz 3.0752
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#625

```
ubr 0.7 2 9.7
umv stx 0.26 sty -1.10900 stz 3.07
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#626

```
ubr 0.6 2 9.6
umv stx 0.2749 sty -1.10900 stz 3.0621
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#627

```
ubr 0.5 2 9.5
umv stx 0.2584 sty -1.10900 stz 3.06063
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 2
```
#628

```
ubr 0.4 2 9.4
umv stx 0.2552 sty -1.10900 stz 3.06024
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#629

```
ubr 0.3 2 9.3
umv stx 0.25 sty -1.10900 stz 3.06024
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#630

```
ubr 0.2 2 9.2
umv stx 0.24015 sty -1.10900 stz 3.05947
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#631

```
ubr 0.1 2 9.1
umv stx 0.23 sty -1.10900 stz 3.058
ascan energy2 A[energy]+.0002 A[energy]-0.0018 400 10
```
#632

2013-07-21

```
ubr 0 2 9.1
umv stx 0.225 sty -1.10900 stz 3.058
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10
```
#664

```
ubr 0 2 9.3
umv stx 0.22 sty -1.10900 stz 3.059
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10
```
#665

```
ubr 0 2 9.7
umv stx 0.1937 sty -1.10900 stz 3.06562
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10
```
#666

```
ubr 0 2 9.9
umv stx 0.17905 sty -1.10900 stz 3.07017
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10
```
#667

```
ubr 1 3 9
umv stx 0.16205 sty -1.10900 stz 3.05014
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #668

ubr 1 2.9 9
umv stx 0.17205 sty -1.10900 stz 3.05014
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #669

ubr 1 2.8 9
umv stx 0.19205 sty -1.10900 stz 3.05014
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #670

ubr 1 2.7 9
umv stx 0.23205 sty -1.10900 stz 3.05014
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #671

ubr 1 2.6 9
umv stx 0.26205 sty -1.10900 stz 3.05014
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #672

ubr 1 2.5 9
umv stx 0.26205 sty -1.10900 stz 3.05014
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #673

ubr 1 2.4 9
umv stx 0.26205 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #674

ubr 1 2.3 9
umv stx 0.26205 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #675

ubr 1 2.2 9
umv stx 0.26205 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #676

ubr 1 2.1 9
umv stx 0.26205 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #677

ubr 1 2 9
umv stx 0.29165 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 2    #678

ubr 1 2 8.9
umv stx 0.29165 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #679

ubr 1 2 8.8
umv stx 0.29165 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #680

ubr 1 2 8.7
umv stx 0.29165 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #683

ubr 1 2 8.6
umv stx 0.29165 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10   #684
```
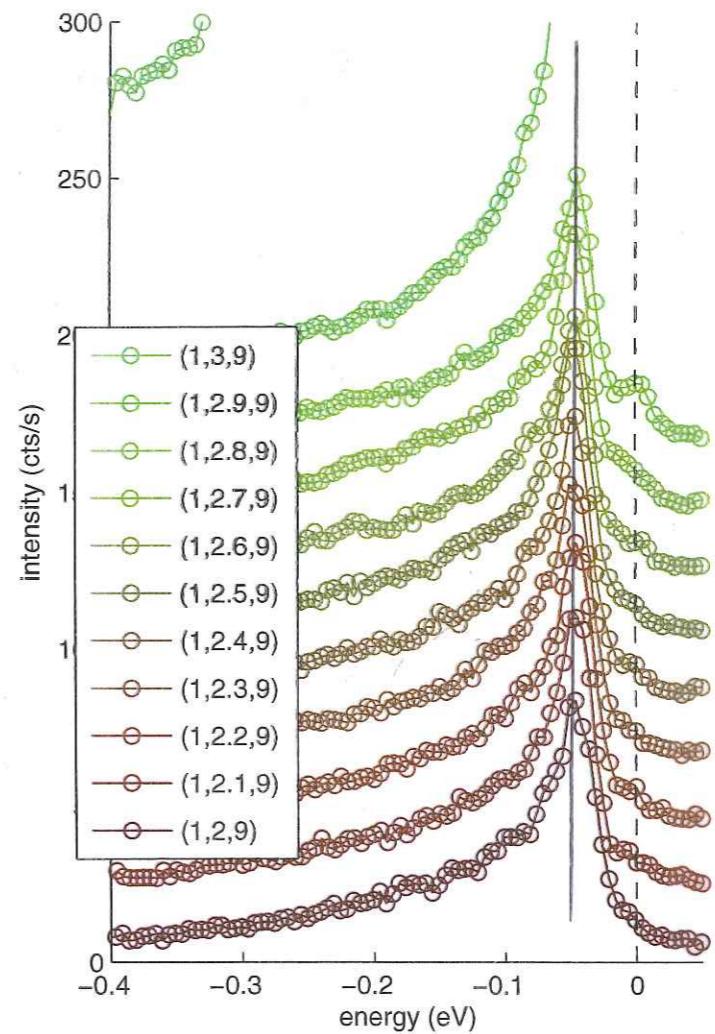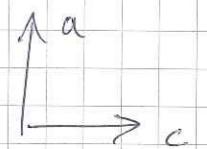

$(1,k,9)$ dispersion 31

no dispersion along b direction

With the above model:

$$\omega_k = 2S\sqrt{\left(J_1^H + J_2^I - J_2^H + J_2^H \cos(kx)\right)^2 - J_1^{H2}\cos^2\left(\frac{k_z}{2}\right)}$$

best fit for $J_1^H = 144$ meV, $J_2^I = 68$ meV, $J_2^H = 2.3$ meV.

```
ubr 1 2 8.5
umv stx 0.29165 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #685

ubr 1 2 8.4
umv stx 0.29165 sty -1.10900 stz 3.04883
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #686

ubr 1 2 8.3
umv stx 0.29165 sty -1.10900 stz 3.0488
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #687

ubr 1 2 8.2
umv stx 0.29165 sty -1.10900 stz 3.0488
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #688

ubr 1 2 8.1
umv stx 0.29165 sty -1.10900 stz 3.0488
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #689

ubr 1 2 8
umv stx 0.29165 sty -1.10900 stz 3.0488
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #690

ubr 1 2 10
umv stx 0.257 sty -1.10900 stz 3.07276
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #700

ubr 1 2 9.9
umv stx 0.307 sty -1.10900 stz 3.06917
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #701

ubr 1 2 9.8
umv stx 0.2716 sty -1.10900 stz 3.07113
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #702

ubr 1 2 9.7
umv stx -0.0535 sty -1.10900 stz 3.05917
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #703

ubr 1 2 9.6
umv stx 0.37735 sty -1.10900 stz 3.04327
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #704

ubr 1 2 9.5
umv stx 0.27885 sty -1.10900 stz 3.06466
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #705

ubr 1 2 9.4
umv stx 0.27985 sty -1.10900 stz 3.06466
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #706

ubr 1 2 9.3
umv stx 0.2794 sty -1.10900 stz 3.06391
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #707

ubr 1.1 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #708
```

```
ubr 1.2 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #709

ubr 1.3 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #710

ubr 1.4 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #711

ubr 1.5 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #712

ubr 1.6 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #713

ubr 1.7 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830

ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #714

ubr 1.8 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #715

ubr 1.9 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #716

ubr 1.95 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 2  #717

ubr 2.1 2 9
umv stx 0.291650 sty -1.10900 stz 3.048830
ascan energy2 A[energy]+.0002 A[energy]-0.0008 200 10  #718
```