Problem 1: Starting a refinement with bad profile coefficients & only an approximate structure is quite hard

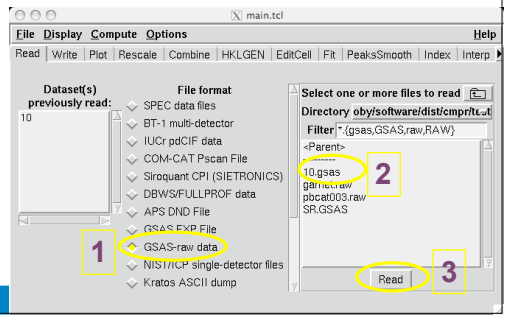
- Solution #1:
  - Collect data using a standard with a known structure
  - Fit the standard (easier since structure & cell can be fixed)
  - Create an instrument parameter file in INSTEDIT specific to the instrument type/conditions (CW only)
- Solution #2:
  - Fit peak widths for selected peaks (in CMPR or RAWPLOT)
  - Fit profile coefficients to peak widths (in CMPR) (CW only)
  - Edit profile terms in refinement or create/edit instrument parameter file in INSTEDIT

Will make use of CMPR program

6

1.0 Peak fitting in CMPR. Step 1: Read in data

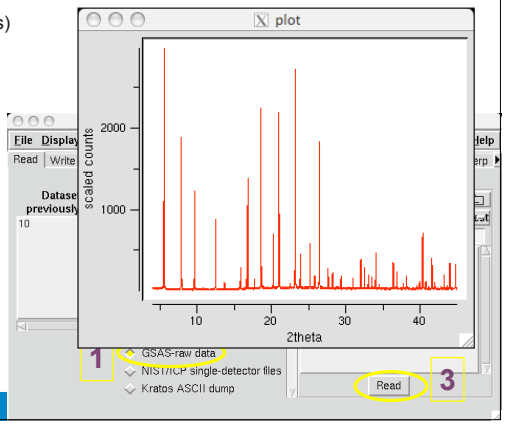
1. Select format
2. Select directory/file(s)
3. Push read button



1.1 Peak fitting in CMPR. Step 1: Read in data

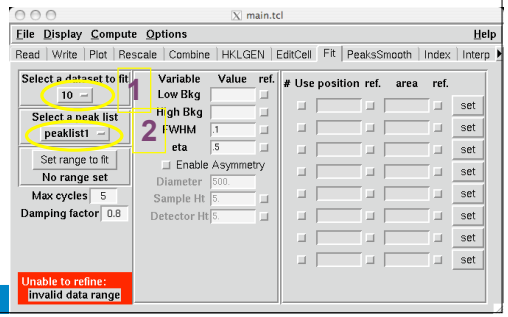
1. Select format
2. Select directory/file(s)
3. Push read button

Data then appear in plot window



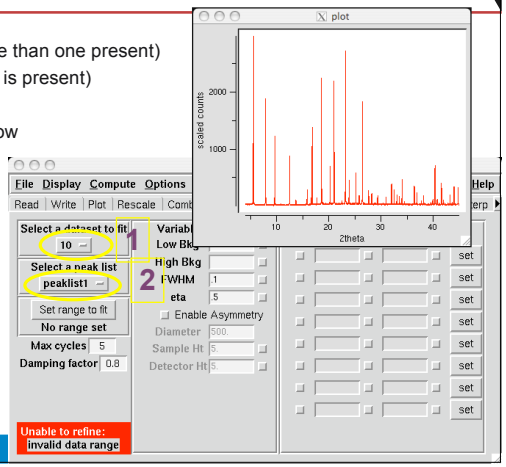
1.2a Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)



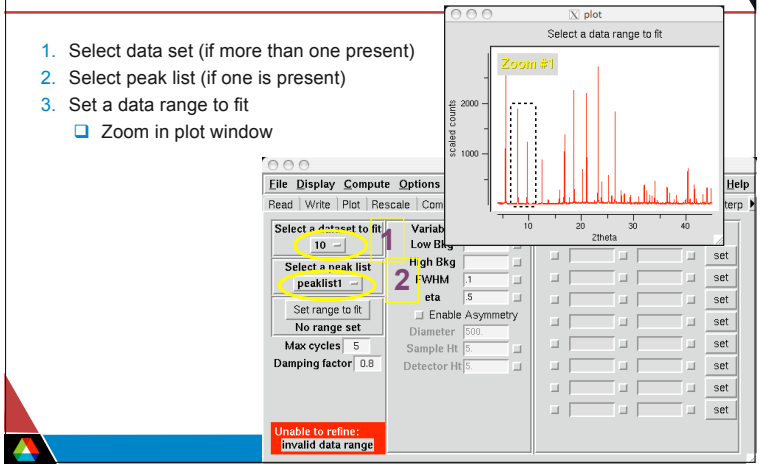
1.2b Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
   - ❑ Zoom in plot window



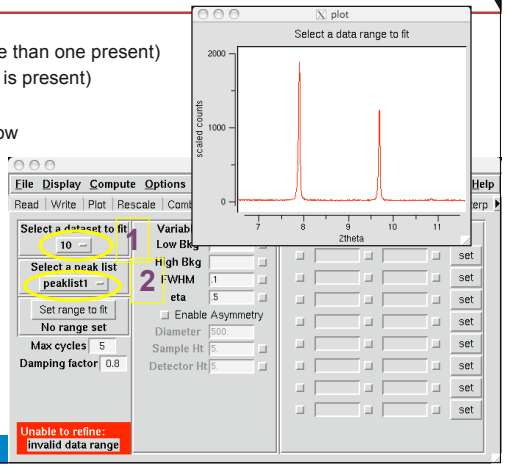
1.2c Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
   - ❑ Zoom in plot window



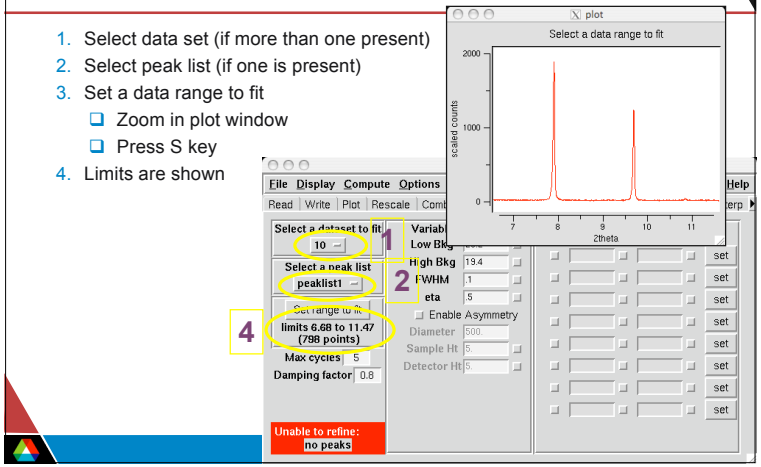
1.2d Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
   - ❑ Zoom in plot window



1.2e Peak fitting in CMPR. Step 2: Select range to fit

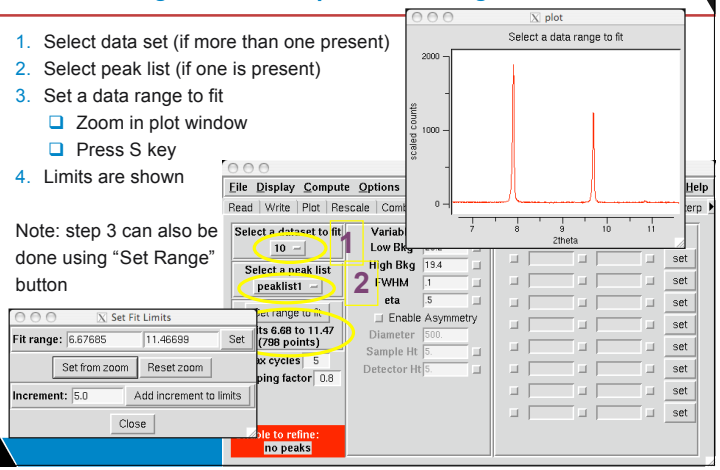
1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
   - ❑ Zoom in plot window
   - ❑ Press S key
4. Limits are shown



1.2f Peak fitting in CMPR. Step 2: Select range to fit

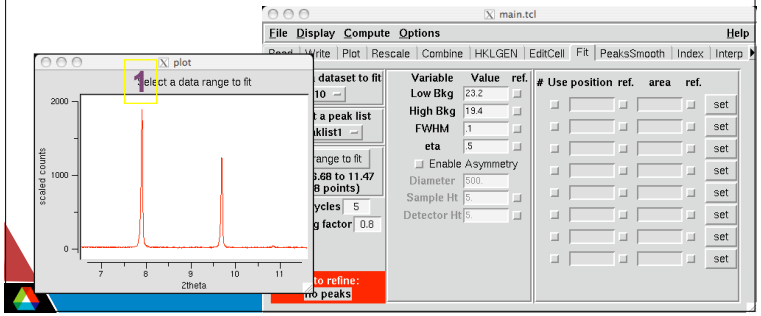
1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
   - Zoom in plot window
   - Press S key
4. Limits are shown

Note: step 3 can also be done using “Set Range” button



1.3a Peak fitting in CMPR. Step 3: Enter Peak Positions

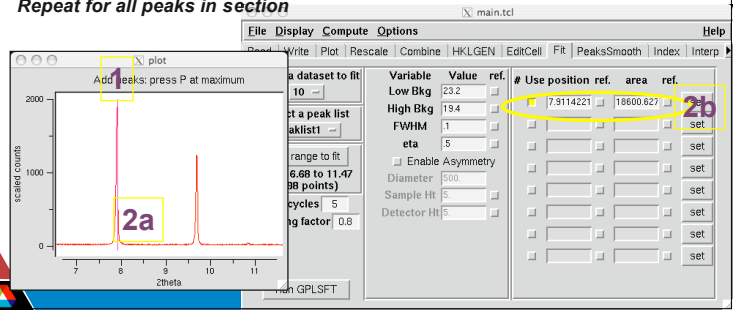
1. Move mouse to peak location
2. Press P key



1.3b Peak fitting in CMPR. Step 3: Enter Peak Positions

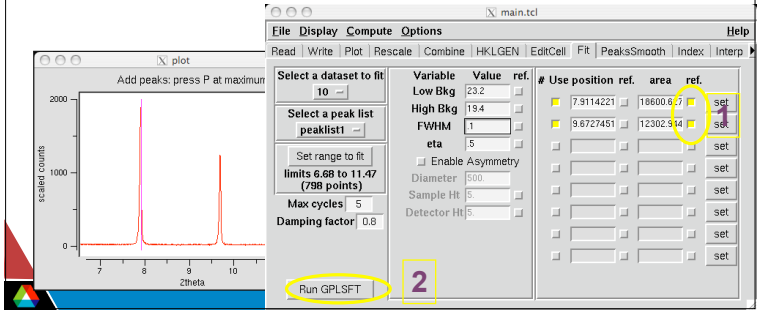
1. Move mouse to peak location
2. Press P key
   a) line appears at peak location
   b) Peak entry appears in table

Repeat for all peaks in section



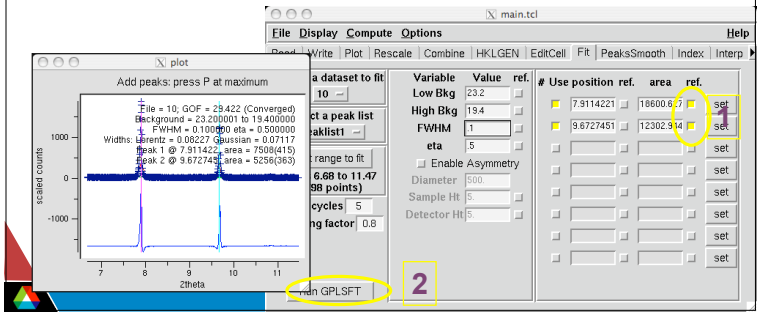
1.4a Peak fitting in CMPR. Step 4A: Start fitting peaks

1. Select peaks areas to be refined
2. Press run GPLS button to perform fit



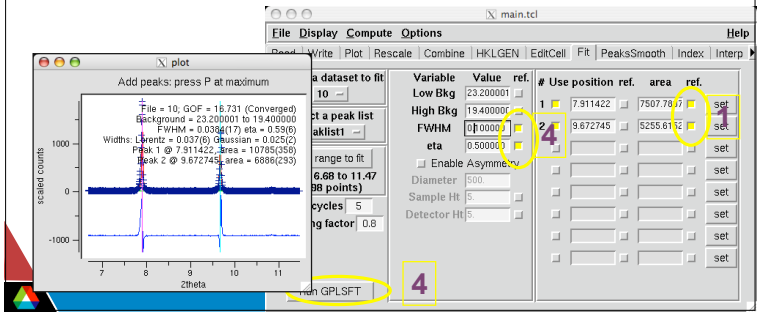
1.4b Peak fitting in CMPR. Step 4A: Start fitting peaks

1. Select peaks areas to be refined
2. Press run GPLS button to perform fit
3. Plot now shows [crummy] fit



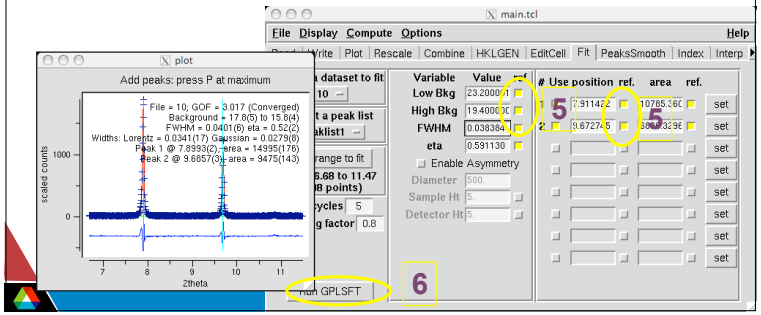
1.4c Peak fitting in CMPR. Step 4A: Start fitting peaks

1. Select peaks areas to be refined
2. Press run GPLS button to perform fit
3. Plot now shows [crummy] fit
4. Refine peak width & shape (Gaussian: eta = 0; Lorentz: eta = 1)



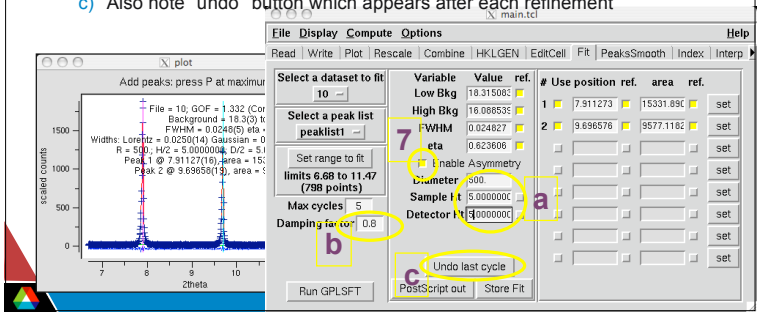
1.4d Peak fitting in CMPR. Step 4B: Continue fitting peaks

5. Select peaks positions & backgrounds to be refined in addition
6. Press run GPLS button to perform fit
7. Plot now shows reasonable fit



1.4e Peak fitting in CMPR. Step 4C: Treat Low-Angle Asymmetry (optional)

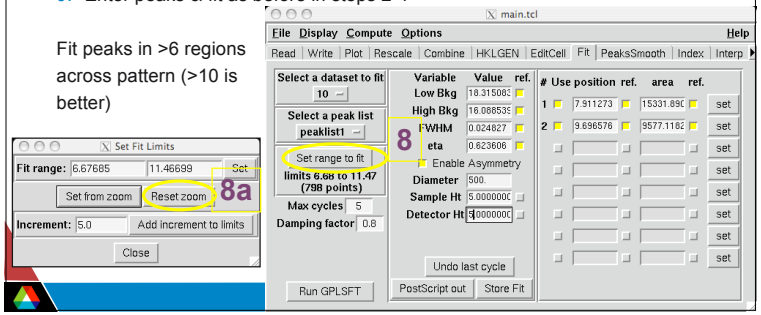
7. Turn on “Enable Asymmetry” & Refine
   a) Don’t refine sample & detector heights -- use measured value
   b) If you have to refine heights; turn off other vars first and/or decrease damping
   c) Also note “undo” button which appears after each refinement



1.4f Peak fitting in CMPR. Step 4D: Continue fitting peaks across pattern

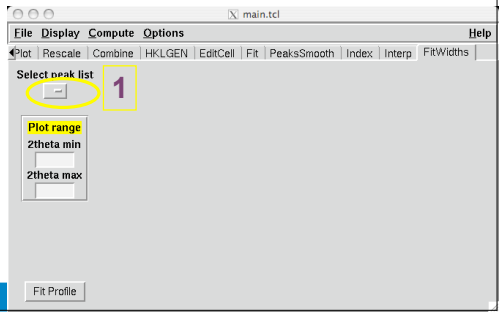
8. Press “Set range to fit” button
   a) Press Reset zoom
   b) Zoom in on a new region to select a small number of peaks
   c) Press “set from zoom” or the “S” key
9. Enter peaks & fit as before in steps 2-4

Fit peaks in >6 regions across pattern (>10 is better)



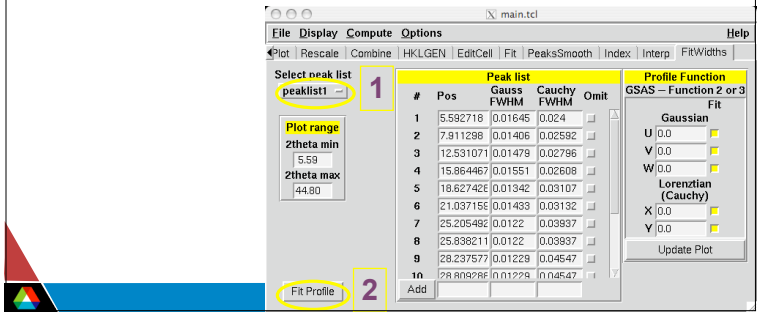
1.5a Fit Profile Coefficients to Peak Widths in CMPR: Use FitWidths

1. Select peak list



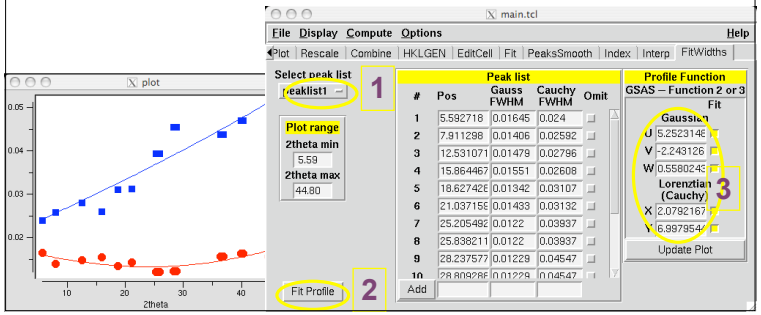
1.5b Fit Profile Coefficients to Peak Widths in CMPR: Use FitWidths

1. Select peak list
2. Press “Fit Profile” button to fit UVW’s



1.5c Fit Profile Coefficients to Peak Widths in CMPR: Use FitWidths

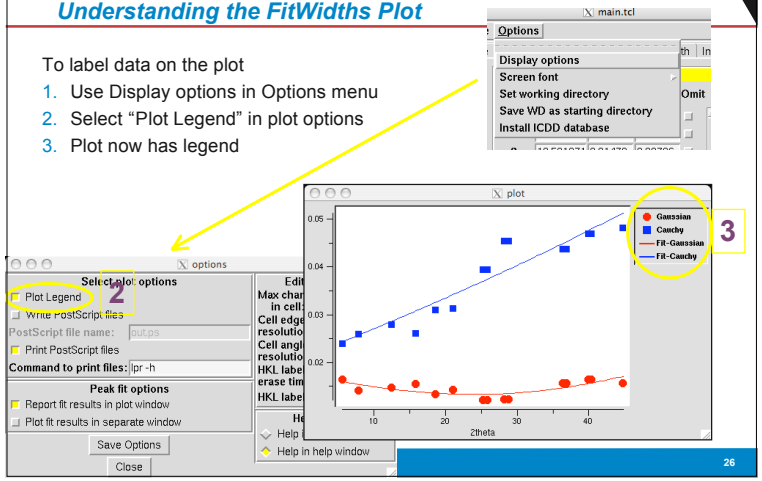
1. Select peak list
2. Press “Fit Profile” button to fit UVW’s
3. Values from fitting appear in boxes; Plot shows fit
4. Write down U,V,W,X & Y values



1.6 Fitted Profile Coefficients in CMPR: Understanding the FitWidths Plot

To label data on the plot

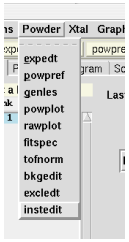
1. Use Display options in Options menu
2. Select “Plot Legend” in plot options
3. Plot now has legend



1.7a Start INSTEDIT from EXPGUI to modify an Instrument Parameter file

There are two ways to start INSTEDIT:

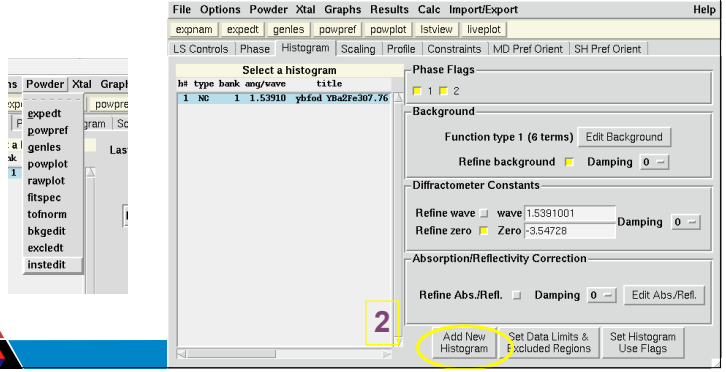
1) from entry in Powder menu bar ***or***



1.7b Start INSTEDIT from EXPGUI to modify an Instrument Parameter file

There are two ways to start INSTEDIT:

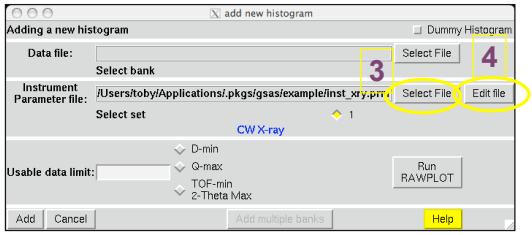
1) from entry in Powder menu bar ***or***
2) Add New Histogram window



1.7c Start INSTEDIT from EXPGUI to modify an Instrument Parameter file

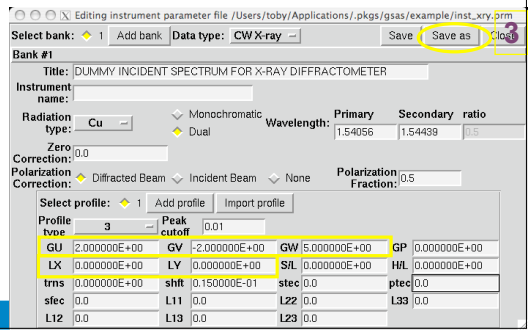
There are two ways to start INSTEDIT:

1) from entry in Powder menu bar ***or***
2) Add New Histogram window
3) Select instrument parameter file to start from
4) Press Edit file to open INSTEDIT



1.8 Use INSTEDIT to modify Instrument Parameter file contents

1) Set U,V & W as GU, GV & GW and X & Y as LX & LY; set GP = 0
2) While you are at it, set wavelength, S/L & H/L etc... to default values
3) Save under a new name



1.9 WIDPLT Tool in EXPGUI Can Be Used to Plot Peak Widths vs 2θ and Compare to Instrumental Resolution

- WIDPLT is EXPGUI Graphs menu

Reference widths are saved in files named widplt_...

Define a few items in this file for each reference:

```
set UVWP(Cu1b) {239.7 -298.2 180.8 0}
set wave(Cu1b) 1.54
set XY(Cu1b) {0 0}
set lblarr(Cu1b) "BT-1 Cu(311) 1b'"
set ttrange(Cu1b) "5 165"
lappend datalist Cu1b
```

(see file example_widplt_BT1)