

successful alignment Co₃Sn₂S₂ no inplane info

Created: 6/11/2025 6:47

Updated: 6/11/2025 10:51

Exported: 6/13/2025 17:53

Prompt:

File: paste.txt

Could you help align my sample? You may use the .env file located at: 'X:\bl17-2\2025_06_Chen\project_roots\Co₃Sn₂S₂\env' for accessing necessary information. When creating a new experiment, use the config_path="X:\bl17-2\2025_06_Chen\project_roots\Co₃Sn₂S₂\config\17_2_config_multigrain_Co₃Sn₂S₂.yaml" as the argument to load correct configuration file.

The experimental operations will completely follow your intention but implemented by human. You will prefix your message Execute Command: [command] to human, and [command] will be typed into the experimental control computer's terminal.

Request one [command] at a time, wait for [command] response before requesting the next [command].

Please pay additional attention to follow instructions, especially for finding the 2nd reference reflection. ⚠ **IMPORTANT: You should remember to do fine scans when the scanned peak is poorly sampled and overly sharp.** ⚠

Be precise and use enough digits (at least 4 digits) when you want to use umv to move motors, as the peaks can be extremely sharp.

You will work with a vertical reflection setup. Make sure you optimize lattice constants when appropriate; for cubic systems, avoid optimizing the lattice constants upon finding the second reference reflection. Before you setlat or or0/or1, always check the detector image first to make sure the peak is well optimized and centered.

⚠️ **CRITICAL:** If you only capture the tail of motor scan instead of the entire peak, you **MUST** extend your scan range to capture the peak accurately. ⚠️

⚠️ **CRITICAL:** If you noticed an offset of any motor, you **MUST** account for this offset value when you use theoretically calculated motor angles when searching for reference reflections. ⚠️

The in-plane orientation of the sample is completely unknown, so you should expect to perform a wider phi scan in the beginning to capture the non-specular peak based on the crystal symmetry. ⚠️
CRITICAL: Please avoid requesting overly wide scan such as phi from -180 to 180 ⚠️

There might be few degrees offsets in motors, and be careful not to recognize hot pixels as peaks. I am attaching two example detector images with and without a peak for your reference. If you do not see a peak at initial search, try starting with increased scan range.

Response:

I'll help you align your sample. Let me start by loading the environment file and setting up the experiment.

load_env

Request

```
{  
  "env_file": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\env"  
}
```

Response

```
{  
  "PROJECT_ROOT": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2"  
}
```

Great! I've loaded the environment file. Now let me create a session for our experiment.

create_session

Request

```
{}
```

Response

Created new session with ID: 6e65513f-2af4-477e-9e35-fe9ba5ab1bd1

Now I'll create an experiment object with the configuration file you specified.

execute_function

Request

```
{
  "store_as": "expt",
  "arguments": "config_path=\"X:\\\\bl17-2\\\\2025_06_Chen\\\\project_roots\\\\Co3Sn2S2",
  "session_id": "6e65513f-2af4-477e-9e35-fe9ba5ab1bd1",
  "function_name": "create_experiment"
}
```

Response

Stored result as 'expt' in session 6e65513f-2af4-477e-9e35-fe9ba5ab1bd1. Result: <llm4x

Excellent! The experiment object has been created. Now let me get the sample information to understand the crystal structure and available peaks.

call_method

Request

```
{
  "arguments": "sort_by='intensity', ascending=False, max_rows=30",
  "session_id": "6e65513f-2af4-477e-9e35-fe9ba5ab1bd1",
  "method_name": "get_sample_information",
  "object_name": "expt"
}
```

Response

Result of `expt.get_sample_information()` in session `6e65513f-2af4-477e-9e35-fe9ba5ab1bd1`

Incident X-ray wavelength: 0.7749 Angstrom

Sample Structure Information

```

Structure Summary:  $\text{Co}_3(\text{SnS})_2$

Lattice

abc : 5.3574 5.3574 13.1274

angles : 90.0000 90.0000 120.0000

volume : 326.2991

A : 5.3574 0.0000 0.0000

B : -2.6787 4.6396 0.0000

C : 0.0000 0.0000 13.1274

pbcs : True True True

```

Diffraction Peak Analysis

Diffraction Data Table

Table contains 29 total rows, sorted by `intensity` in descending order.

#	tth	intensity	d_hkl	theta_minus_rel_angle	hkl indices
---	----	-----	-----	-----	-----
1	20.4004	37.0756	2.1879	10.2002	[0 0 6]
2	10.1597	26.7452	4.3758	5.0798	[0 0 3]
3	52.9341	9.7012	0.8693	4.4585	[0 -2 14]
4	52.9341	9.7012	0.8693	4.4585	[2 0 14]
5	52.9341	9.7012	0.8693	4.4585	[-2 2 14]
6	35.7249	7.1978	1.2632	2.0641	[-1 1 10]
7	35.7249	7.1978	1.2632	2.0641	[1 0 10]
8	35.7249	7.1978	1.2632	2.0641	[0 -1 10]
9	41.4859	4.2287	1.0939	20.7429	[0 0 12]
10	30.8090	3.9315	1.4586	15.4045	[0 0 9]
11	49.8661	3.7299	0.9191	13.5075	[1 -1 14]
12	49.8661	3.7299	0.9191	13.5075	[0 1 14]
13	49.8661	3.7299	0.9191	13.5075	[-1 0 14]
14	44.9862	3.4488	1.0128	0.2785	[-2 1 12]
15	44.9862	3.4488	1.0128	0.2785	[2 -1 12]
16	44.9862	3.4488	1.0128	0.2785	[1 -2 12]
17	44.9862	3.4488	1.0128	0.2785	[-1 2 12]
18	44.9862	3.4488	1.0128	0.2785	[1 1 12]

19	44.9862	3.4488	1.0128	0.2785	[-1 -1 12]
20	49.4755	1.7922	0.9259	1.2146	[-2 0 13]
21	49.4755	1.7922	0.9259	1.2146	[0 2 13]
22	49.4755	1.7922	0.9259	1.2146	[2 -2 13]
23	39.1729	1.1225	1.1558	5.1616	[0 1 11]
24	39.1729	1.1225	1.1558	5.1616	[-1 0 11]
25	39.1729	1.1225	1.1558	5.1616	[1 -1 11]
26	52.5551	0.3387	0.8752	26.2775	[0 0 15]
27	46.2418	0.0470	0.9867	10.8422	[0 -1 13]
28	46.2418	0.0470	0.9867	10.8422	[1 0 13]
29	46.2418	0.0470	0.9867	10.8422	[-1 1 13]

Summary Statistics

Key Values

Statistic	tth	intensity	d_hkl
:-----	:-----	:-----	:-----
min	10.1597	0.0470	0.8693
max	52.9341	37.0756	4.3758
mean	42.9508	5.6477	1.1872

Column Descriptions

- **tth**: Two-theta angle (in degrees)
- **intensity**: Relative intensity of the diffraction peak
- **d_hkl**: Interplanar spacing (in Angstroms)
- **hkl indices**: Miller indices representing structural peaks [h k l]

_Note: This data combines the crystal structure parameters with calculated diffraction

Perfect! I can see this is a Co₃Sn₂S₂ sample with hexagonal structure (space group symmetry based on the lattice parameters: a=b=5.3574 Å, c=13.1274 Å, α=β=90°, γ=120°).

Let me first check the current motor positions to understand our starting point.

Execute Command: wm phi chi eta del mu nu

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 30  
}
```

Response

```

{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",
  "lines_requested": 30,
  "lines_returned": 30,
  "log_lines": [
    "",
    "1391.PSIC> ",
    "",
    "",
    "1391.PSIC> ",
    "",
    "",
    "1391.PSIC> ",
    "",
    "",
    "1391.PSIC> ",
    "",
    "",
    "1391.PSIC> ",
    "",
    "",
    "1391.PSIC> wm hi chi eta del mu nu",
    "Invalid motor:  \"hi\".",
    "",
    "",
    "1392.PSIC> wm phi chi eta del mu nu",
    "",
    "
          phi      chi      eta      del      mu      nu ",
    "
          phi      chi      eta      del      mu      nu ",
    "User",
    " High      105.50000  185.00000  33.01773  68.17637   0.50000  29.18834 ",
    " Current      0.00000  90.00000   0.00000  50.00000  -0.00000   0.00000 ",
    " Low       -279.50000  85.00000  -3.93227  -3.82363  -0.50000 -12.81166 ",
    "Dial",
    " High      195.50000  185.00000  33.76373  65.37639   0.90107  29.18834 ",
    " Current      90.00000  90.00000   0.74600  47.20002   0.40107   0.00000 ",
    " Low       -189.50000  85.00000  -3.18627  -6.62361  -0.09893 -12.81166 ",
    ""
  ],
  "file_size_bytes": 3654990,
  "last_modified_timestamp": 1749649707.7247727,
  "message": "Successfully read 30 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\

```

Good! I can see the current motor positions:

- $\phi = 0.0000^\circ$
- $\chi = 90.0000^\circ$ (vertical reflection geometry)
- $\eta = 0.0000^\circ$
- $\delta = 50.0000^\circ$
- $\mu = -0.0000^\circ$
- $\nu = 0.0000^\circ$

We're in vertical reflection geometry ($\chi = 90^\circ$). Now let me check the current HKL position to see if we have any orientation matrix set.

Execute Command: wh

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 20  
}
```

Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 20,
  "lines_returned": 20,
  "log_lines": [
    "User",
    " High      105.50000  185.00000   33.01773   68.17637    0.50000   29.18834 ",
    " Current      0.00000   90.00000    0.00000   50.00000   -0.00000    0.00000 ",
    " Low       -279.50000   85.00000   -3.93227   -3.82363   -0.50000  -12.81166 ",
    "Dial",
    " High      195.50000  185.00000   33.76373   65.37639    0.90107   29.18834 ",
    " Current      90.00000   90.00000    0.74600   47.20002    0.40107    0.00000 ",
    " Low       -189.50000   85.00000   -3.18627   -6.62361   -0.09893  -12.81166 ",
    "",
    "",
    "1393.PSIC> wh",
    "",
    "H K L =  2.031  0.029136  13.122\t Lambda = 0.7749 Two Theta = 50",
    "",
    "   Alpha      Beta      Psi      Tau      Qaz      Naz      Omega",
    "  32.5739  -21.3406  120.5803   78.0873   90.0000 -178.4161  -25.0000",
    "",
    "      del      eta      chi      phi      nu      mu ",
    "  50.00000    0.00000   90.00000    0.00000    0.00000    0.00000 ",
    ""
  ],
  "file_size_bytes": 3655348,
  "last_modified_timestamp": 1749649774.7458403,
  "message": "Successfully read 20 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
}
```

I see there's already an orientation matrix set (H K L = 2.031, 0.029136, 13.122), but this doesn't seem like a proper alignment. We need to start fresh and find proper reference reflections.

For a hexagonal $\text{Co}_3\text{Sn}_2\text{S}_2$ sample with $c \gg a, b$ ($c=13.1274 \text{ \AA}$ vs $a=b=5.3574 \text{ \AA}$), the c-axis is likely the surface normal. Let's start by finding a specular (0,0,L) reflection.

Looking at the peak table, the strongest (0,0,L) peaks are:

1. (0,0,6) at $2\theta = 20.4004^\circ$ (strongest, 37% intensity)
2. (0,0,3) at $2\theta = 10.1597^\circ$ (second strongest, 26.7% intensity)

Let's start with (0,0,6) since it has the highest intensity. For vertical geometry:

- $\eta \approx \theta = 10.2002^\circ$
- $\delta \approx 2\theta = 20.4004^\circ$

Let me move to these positions:

Execute Command: umv eta 10.2002 del 20.4004

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 20  
}
```

Response

```

{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 20,
  "lines_returned": 20,
  "log_lines": [
    " 10.20020 28.17416 ",
    " 10.20020 27.59801 ",
    " 10.20020 26.99254 ",
    " 10.20020 26.39738 ",
    " 10.20020 25.82051 ",
    " 10.20020 25.22479 ",
    " 10.20020 24.62973 ",
    " 10.20020 24.05289 ",
    " 10.20020 23.45717 ",
    " 10.20020 22.86162 ",
    " 10.20020 22.26596 ",
    " 10.20020 21.66035 ",
    " 10.20020 21.06512 ",
    " 10.20020 20.50752 ",
    " 10.20020 20.38086 ",
    " 10.20020 20.40039 ",
    " 10.20020 20.40039 ",
    " 10.20020 20.40039 ",
    "",
    ""
  ],
  "file_size_bytes": 3656656,
  "last_modified_timestamp": 1749649827.793688,
  "message": "Successfully read 20 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}

```

Good, the motors have moved. Let me check the current position:

Execute Command: wh

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 20  
}
```

Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 20,
  "lines_returned": 20,
  "log_lines": [
    " 10.20020 21.66035 ",
    " 10.20020 21.06512 ",
    " 10.20020 20.50752 ",
    " 10.20020 20.38086 ",
    " 10.20020 20.40039 ",
    " 10.20020 20.40039 ",
    " 10.20020 20.40039 ",
    "",
    "",
    "",
    "1395.PSIC> wh",
    "",
    "H K L = -0.022896 -0.037947 6.0096\t Lambda = 0.7749 Two Theta = 20.4",
    "",
    "   Alpha      Beta      Psi      Tau      Qaz      Naz      Omega",
    " 31.7189 -32.2763 122.5838 91.3347 90.0000 -172.0081 0.0000",
    "",
    "   del      eta      chi      phi      nu      mu ",
    " 20.40039 10.20020 90.00000 0.00000 0.00000 0.00000 ",
    ""
  ],
  "file_size_bytes": 3657021,
  "last_modified_timestamp": 1749649864.80428,
  "message": "Successfully read 20 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
}
```

Perfect! We're now at $\eta = 10.20020^\circ$ and $\delta = 20.40039^\circ$, and the HKL values show we're very close to (0,0,6). Now let's take a detector image to see if we can see the peak:

Execute Command: `pd exposure test_006_initial 1.0`

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 20  
}
```

Response

```

{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 20,
  "lines_returned": 20,
  "log_lines": [
    "# Direct Beam Pixel at TTH/DEL = 0 and GAM/NU = 0:",
    "PD_X_0 =   ; PD_Y_0 =   ",
    "",
    "# Regions of interest",
    "ROI_1_X1=279; ROI_1_Y1=97; ROI_1_X2=279; ROI_1_Y2=97;",
    "ROI_2_X1=277; ROI_2_Y1=95; ROI_2_X2=281; ROI_2_Y2=99;",
    "ROI_3_X1=274; ROI_3_Y1=92; ROI_3_X2=284; ROI_3_Y2=102;",
    "ROI_4_X1=269; ROI_4_Y1=87; ROI_4_X2=289; ROI_4_Y2=107;",
    "ROI_5_X1=79; ROI_5_Y1=1; ROI_5_X2=479; ROI_5_Y2=193;",
    "ROI_6_X1=179; ROI_6_Y1=96; ROI_6_X2=379; ROI_6_Y2=98;",
    "ROI_7_X1=277; ROI_7_Y1=7; ROI_7_X2=279; ROI_7_Y2=187;",
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;"
  ],
  "file_size_bytes": 3658889,
  "last_modified_timestamp": 1749649897.8158083,
  "message": "Successfully read 20 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}

```

Good, I can see the ROI definitions. Now let me check if the image file was created and visualize it:

explore_directory

Request

```
{  
  "max_depth": 1,  
  "show_recent": null,  
  "file_pattern": "*.raw",  
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"  
}
```

Response

Error executing code: Cannot convert undefined or null to object

Let me try with the default show_recent parameter:

explore_directory

Request

```
{  
  "max_depth": 1,  
  "file_pattern": "*.raw",  
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"  
}
```

Response

Directory scan for: X:\bl17-2\2025_06_Chen\project_roots\Co3Sn2S2\images
Scan time: 2025-06-11 06:52:03

 images

-  003_initial_061125-032459.raw (1.1 MB), modified 3 hours ago
-  006_eta_centered_061125-044426.raw (1.1 MB), modified 1 hour ago
-  006_eta_optimized_061125-025321.raw (1.1 MB), modified 3 hours ago
-  006_final_061125-040903.raw (1.1 MB), modified 2 hours ago
-  006_final_optimized_061125-031948.raw (1.1 MB), modified 3 hours ago
-  006_final_optimized_061125-050052.raw (1.1 MB), modified 1 hour ago
-  006_final_optimized_061125-060916.raw (1.1 MB), modified 27 minutes ago
-  006_initial_061125-024503.raw (1.1 MB), modified 3 hours ago
-  006_initial_061125-034550.raw (1.1 MB), modified 2 hours ago
-  006_initial_061125-044109.raw (1.1 MB), modified 1 hour ago
-  0114_initial_061125-041319.raw (1.1 MB), modified 2 hours ago
-  011_initial_061125-033022.raw (1.1 MB), modified 3 hours ago
-  1010_final_optimized_061125-052442.raw (1.1 MB), modified 1 hour ago
-  1010_initial_061125-051129.raw (1.1 MB), modified 1 hour ago
-  initial_006_search_061125-055400.raw (1.1 MB), modified 43 minutes ago
-  initial_check_061125-005204.raw (1.1 MB), modified 5 hours ago
-  optimized_006_061125-010814.raw (1.1 MB), modified 5 hours ago
-  search_006_061125-005441.raw (1.1 MB), modified 5 hours ago
-  search_1014_061125-011920.raw (1.1 MB), modified 5 hours ago
-  test_006_initial_061125-062853.raw (1.1 MB), modified 8 minutes ago

===== RECENT FILES =====

Most recent *.raw files:

-  test_006_initial_061125-062853.raw (modified: 2025-06-11 06:43:49)
-  006_final_optimized_061125-060916.raw (modified: 2025-06-11 06:24:13)
-  initial_006_search_061125-055400.raw (modified: 2025-06-11 06:08:57)
-  1010_final_optimized_061125-052442.raw (modified: 2025-06-11 05:39:39)
-  1010_initial_061125-051129.raw (modified: 2025-06-11 05:26:25)

Great! I can see the test_006_initial_061125-062853.raw file was created. Let me visualize it:

read_and_plot_image

Request

```
{  
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\test_006_in  
}
```



I don't see a clear peak in the detector image. Let me do a broad eta scan to locate the peak. Since we're looking for the (0,0,6) peak and there might be a few degrees offset in the motors, I'll do a wider eta scan:

Execute Command: dscan eta -2 2 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

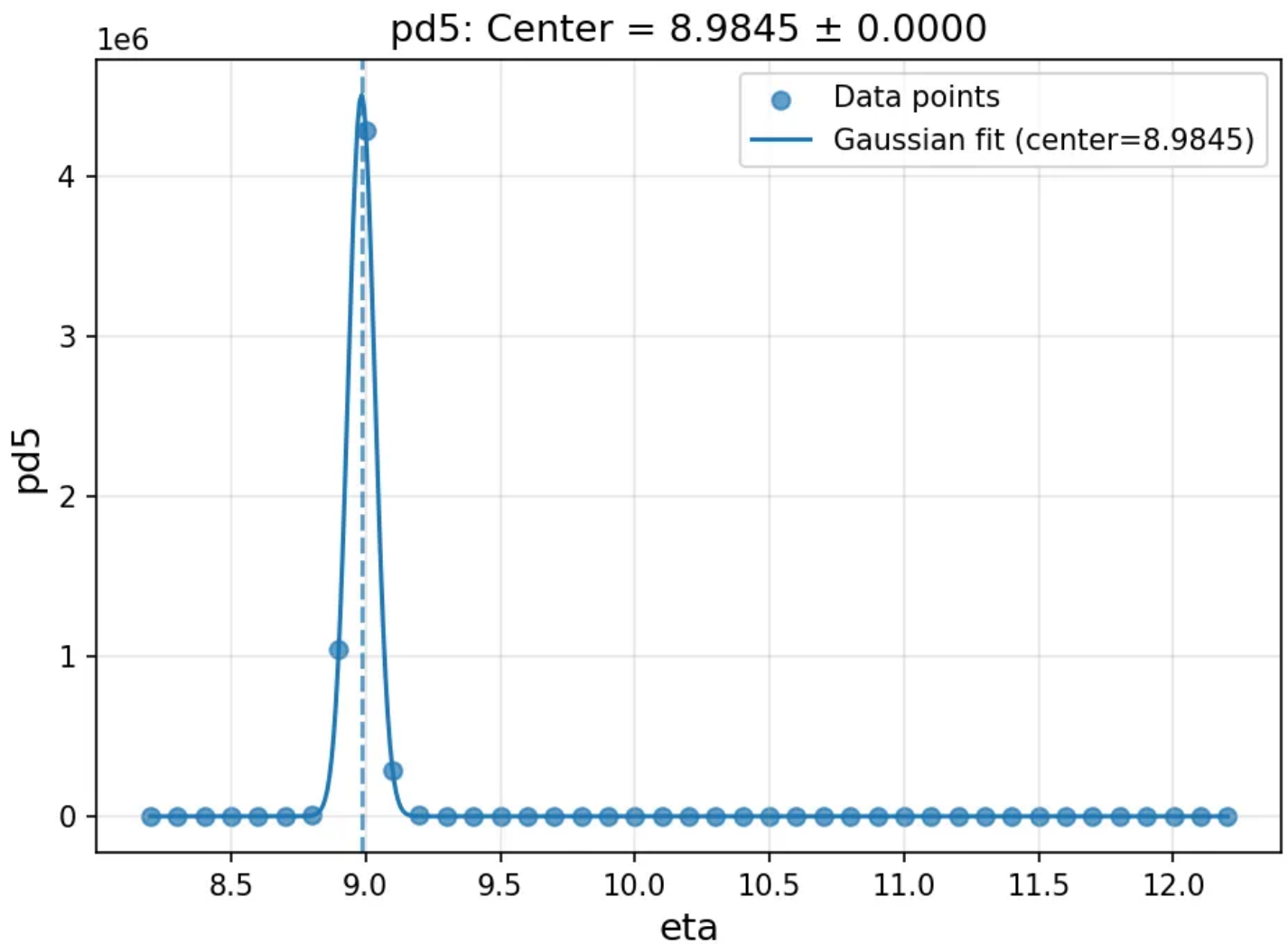
```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    " 39, 12.1002, 0.5000, 0.78722, 0.00042, 0.00561, 0.00483, 0,
    \"Shutter open.\",
    \"Shutter closed.\",
    \" 40 12.2002 0.5 0.5 0.5 0.7874 0.00043 0.00553 0.00486
    \"12.200195 -0.094874688 -0.041772017 6.0016311 20564.166 0.78739 0.00043 0.00553 0.
    \" 40, 12.2002, 0.5000, 0.78739, 0.00043, 0.00553, 0.00486, 0,
    \"/home/det/p2_det/images/mpy_spec_scan69*\",
    \"\",
    \"Returning eta to 10.2002\",
    \"\",
  ],
  "file_size_bytes": 3701644,
  "last_modified_timestamp": 1749649993.888345,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```

Good! The scan is complete and eta has returned to 10.2002. Now let me visualize the scan results to see if we can find the peak:

read_and_plot_spec

Request

```
{
  "fit_type": "gaussian",
  "x_column": "eta",
  "y_columns": "pd5",
  "scan_number": "69",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"
}
```



Excellent! I found a sharp peak centered at $\eta = 8.9845^\circ$. This shows there's about a 1.22° offset from the expected η value ($10.2002^\circ - 8.9845^\circ \approx 1.22^\circ$). Let me move η to the peak center:

Execute Command: `umv eta 8.9845`

Prompt:

Please read the log and continue.

Response:

`read_log`

Request

```
{
  "lines": 15
}
```

Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "Returning eta to 10.2002",
    "",
    "",
    "1398.PSIC> umv eta 8.9845",
    "",
    "      eta ",
    " 10.18684 ",
    "  9.38119 ",
    "  8.94543 ",
    "  8.94543 ",
    "  8.98449 ",
    "  8.98449 ",
    "  8.98449 ",
    "",
    ""
  ],
  "file_size_bytes": 3701770,
  "last_modified_timestamp": 1749650045.9071772,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
}
```

Good, eta has moved to 8.98449°. Now I need to check if the peak is centered in the detector. Let me take another image:

Execute Command: pd exposure 006_eta_centered 1.0

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "ROI_7_X1=277; ROI_7_Y1=7; ROI_7_X2=279; ROI_7_Y2=187;",  
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",  
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",  
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",  
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",  
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",  
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",  
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",  
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",  
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;"  
  ],  
  "file_size_bytes": 3703679,  
  "last_modified_timestamp": 1749650095.9249763,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Now let me visualize the detector image:

read_and_plot_image

Request

```
{
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\006_eta_cen
}
```

Response

```
{
  "status": "error",
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\006_eta_cen
  "error": "Image file not found: X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\im
  "error_type": "FileNotFoundError",
  "message": "Failed to read and plot image: Image file not found: X:\\bl17-2\\2025_06_
}
```

Let me check what files are available:

explore_directory

Request

```
{
  "max_depth": 1,
  "file_pattern": "006_eta_centered*.raw",
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"
}
```

Response

Directory scan for: X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images

Scan time: 2025-06-11 06:56:14

 images

===== RECENT FILES =====

Let me check the most recent files:

explore_directory

Request

```
{  
  "max_depth": 1,  
  "show_recent": true,  
  "file_pattern": "*.raw",  
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"  
}
```

Response

Directory scan for: X:\bl17-2\2025_06_Chen\project_roots\Co3Sn2S2\images
Scan time: 2025-06-11 06:56:20

 images

-  003_initial_061125-032459.raw (1.1 MB), modified 3 hours ago
-  006_eta_centered_061125-044426.raw (1.1 MB), modified 1 hour ago
-  006_eta_centered_061125-063210.raw (1.1 MB), modified 9 minutes ago
-  006_eta_optimized_061125-025321.raw (1.1 MB), modified 3 hours ago
-  006_final_061125-040903.raw (1.1 MB), modified 2 hours ago
-  006_final_optimized_061125-031948.raw (1.1 MB), modified 3 hours ago
-  006_final_optimized_061125-050052.raw (1.1 MB), modified 1 hour ago
-  006_final_optimized_061125-060916.raw (1.1 MB), modified 32 minutes ago
-  006_initial_061125-024503.raw (1.1 MB), modified 3 hours ago
-  006_initial_061125-034550.raw (1.1 MB), modified 2 hours ago
-  006_initial_061125-044109.raw (1.1 MB), modified 2 hours ago
-  0114_initial_061125-041319.raw (1.1 MB), modified 2 hours ago
-  011_initial_061125-033022.raw (1.1 MB), modified 3 hours ago
-  1010_final_optimized_061125-052442.raw (1.1 MB), modified 1 hour ago
-  1010_initial_061125-051129.raw (1.1 MB), modified 1 hour ago
-  initial_006_search_061125-055400.raw (1.1 MB), modified 47 minutes ago
-  initial_check_061125-005204.raw (1.1 MB), modified 5 hours ago
-  optimized_006_061125-010814.raw (1.1 MB), modified 5 hours ago
-  search_006_061125-005441.raw (1.1 MB), modified 5 hours ago
-  search_1014_061125-011920.raw (1.1 MB), modified 5 hours ago
-  test_006_initial_061125-062853.raw (1.1 MB), modified 12 minutes ago

===== RECENT FILES =====

Most recent *.raw files:

-  006_eta_centered_061125-063210.raw (modified: 2025-06-11 06:47:07)
-  test_006_initial_061125-062853.raw (modified: 2025-06-11 06:43:49)
-  006_final_optimized_061125-060916.raw (modified: 2025-06-11 06:24:13)
-  initial_006_search_061125-055400.raw (modified: 2025-06-11 06:08:57)
-  1010_final_optimized_061125-052442.raw (modified: 2025-06-11 05:39:39)

I see the file 006_eta_centered_061125-063210.raw. Let me visualize it:

read_and_plot_image

Request

```
{  
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\006_eta_cen  
}
```



Great! I can see a real diffraction peak in the detector image. It appears as a broad intensity distribution (not just hot pixels) and is already quite well centered. Now I need to optimize its position by scanning chi and del. Let me start with a chi scan:

Execute Command: dscan chi -1 1 20 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    " 19,      90.9,    0.5000,  0.79027,  0.00036,  0.00551,  0.00498,      0,
    \"Shutter open.\",
    \"Shutter closed.\",
    \" 20  91.0000      0.5      0.5      0.5  0.7922  0.0004  0.00549  0.00498
    \"91 0.043895347 -0.078269852 6.0083838 20803.355 0.79215 0.0004 0.00549 0.00498 0 0
    \" 20,      91,    0.5000,  0.79215,  0.0004,  0.00549,  0.00498,      0,
    \"/home/det/p2_det/images/mpy_spec_scan70*\",
    \"\",
    \"Returning chi to 90\",
    \"\",
  ],
  "file_size_bytes": 3727430,
  "last_modified_timestamp": 1749650231.991147,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```

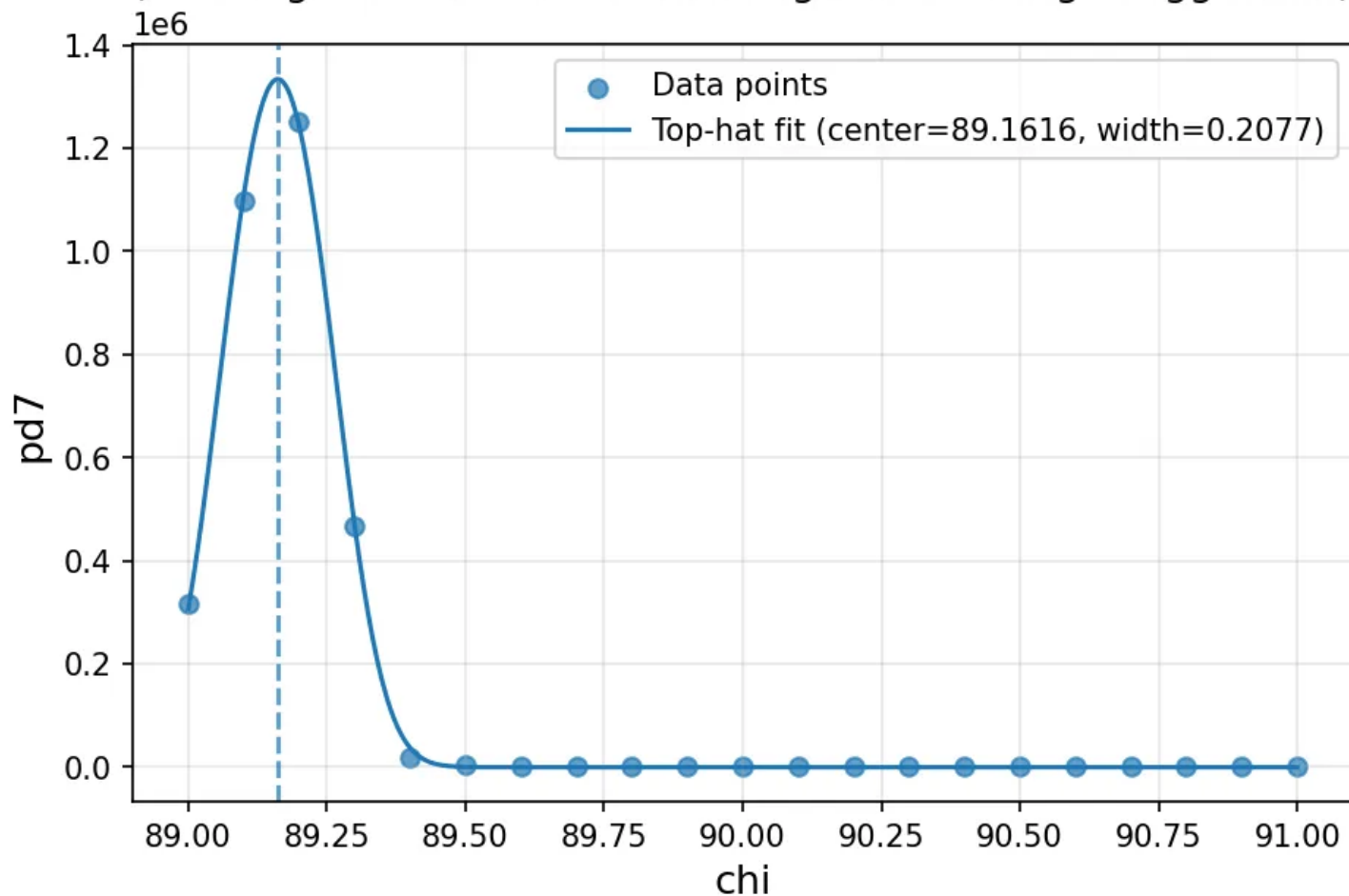
Good, the chi scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{
  "fit_type": "tophat",
  "x_column": "chi",
  "y_columns": "pd7",
  "scan_number": "70",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"
}
```

pd7: Center = 89.1616 ± 0.0005 , Width = 0.2077
(Warning: Fit center near data edge; wider range suggested.)



I see the peak is centered at $\text{chi} = 89.1616^\circ$. The fit shows a warning about being near the data edge, and I notice we're capturing the tail of the peak. Let me do a wider chi scan to capture the full peak:

Execute Command: `dscan chi -2 0 40 0.5`

Prompt:

Please read the log and continue.

Response:

`read_log`

Request

```
{
  "lines": 10
}
```

Response

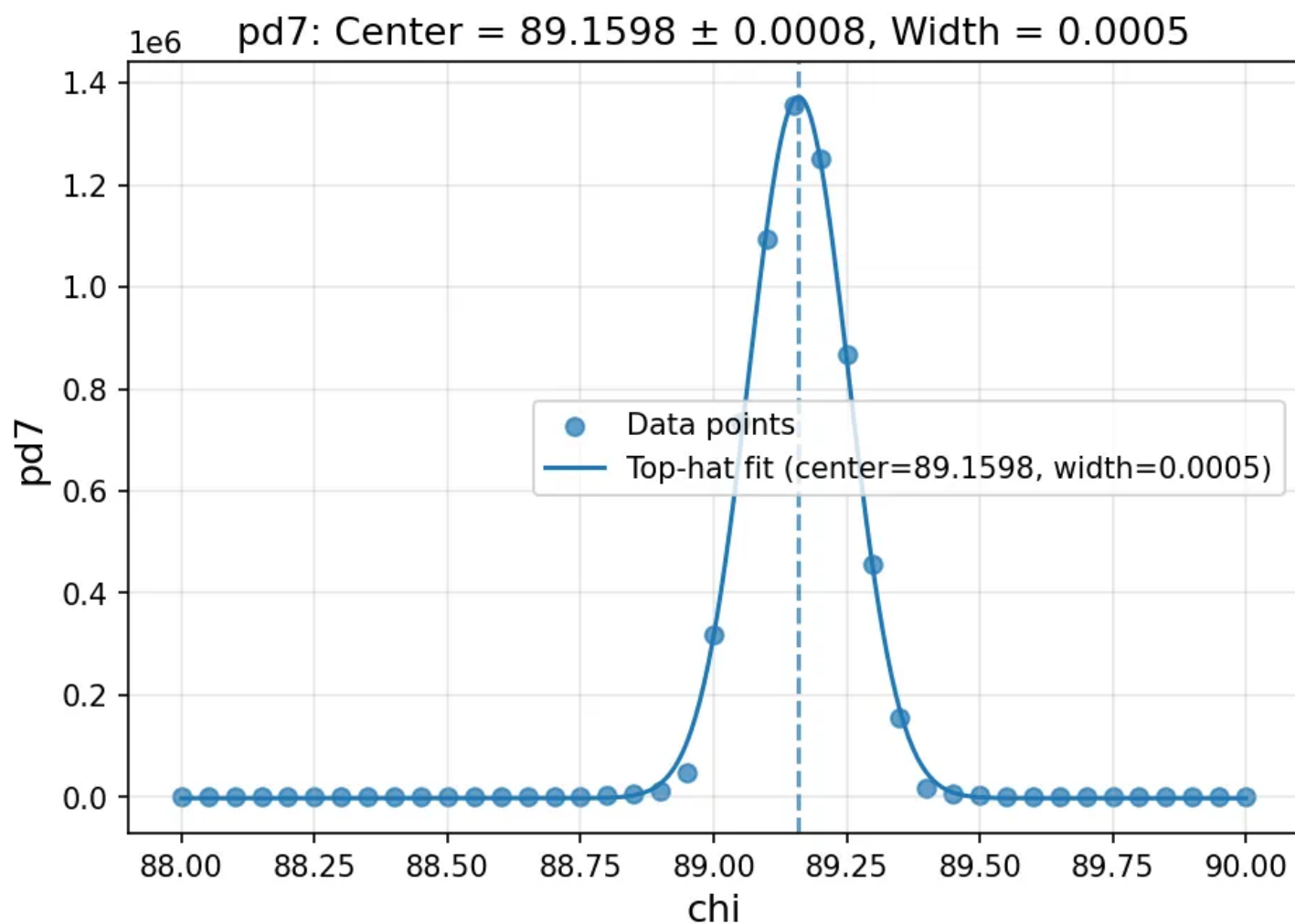
```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "89.95 0.019725268 -0.033464954 6.0109034 20891.337 0.78887 0.00043 0.00568 0.00492",
    " 39,      89.95,    0.5000,   0.78887,   0.00043,   0.00568,   0.00492,        0,",
    "Shutter open.",
    "Shutter closed.",
    " 40   90.0000      0.5      0.5      0.5   0.7858  0.00049  0.00568  0.00492",
    "90 0.020876105 -0.035598912 6.0108291 20892.216 0.78581 0.00049 0.00568 0.00492 0",
    " 40,      90,    0.5000,   0.78581,   0.00049,   0.00568,   0.00492,        0,",
    "/home/det/p2_det/images/mpy_spec_scan71*",
    "",
    ""
  ],
  "file_size_bytes": 3770785,
  "last_modified_timestamp": 1749650320.2015543,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
}
```

The scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{
  "fit_type": "tophat",
  "x_column": "chi",
  "y_columns": "pd7",
  "scan_number": "71",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"
}
```



Perfect! Now I have a complete peak profile centered at $\text{chi} = 89.1598^\circ$. Let me move chi to this position:

Execute Command: `umv chi 89.1598`

Prompt:

Please read the log and continue.

Response:

`read_log`

Request

```
{
  "lines": 10
}
```

Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "",
    "      chi ",
    " 89.98648 ",
    " 89.27975 ",
    " 89.14027 ",
    " 89.15980 ",
    " 89.15980 ",
    " 89.15980 ",
    "",
    ""
  ],
  "file_size_bytes": 3770900,
  "last_modified_timestamp": 1749650353.214081,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
}
```

Good, chi is now at 89.15980°. Now let me scan del to center the peak vertically:

Execute Command: dscan del -1 1 20 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

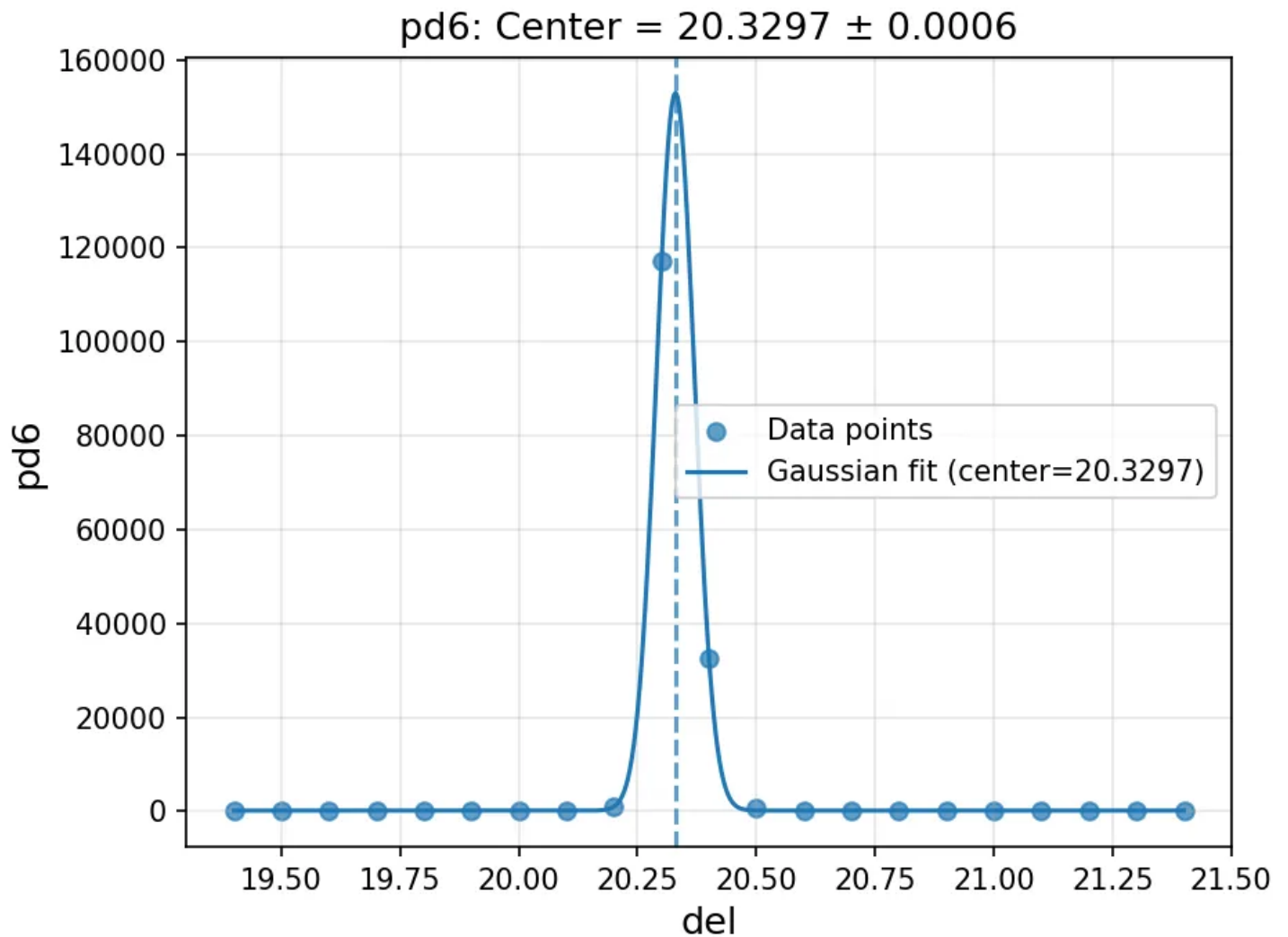
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 19, 21.3004, 0.5000, 0.78363, 0.0004, 0.00555, 0.00489, 0,  
    \"Shutter open.\",  
    \"Shutter closed.\",  
    " 20 21.4004 0.5 0.5 0.5 0.7849 0.00043 0.00548 0.00489  
    \"21.400391 0.020493137 0.0012842375 6.3025072 20970.449 0.78485 0.00043 0.00548 0.0  
    \" 20, 21.4004, 0.5000, 0.78485, 0.00043, 0.00548, 0.00489, 0,  
    \"/home/det/p2_det/images/mpy_spec_scan72*\",  
    \"\",  
    \"Returning del to 20.4004\",  
    \"\",  
  ],  
  "file_size_bytes": 3794798,  
  "last_modified_timestamp": 1749650399.3178165,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

The del scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{
  "fit_type": "gaussian",
  "x_column": "del",
  "y_columns": "pd6",
  "scan_number": "72",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"
}
```



Excellent! The peak is well-centered at $\text{del} = 20.3297^\circ$. This is very close to the expected value of 20.4004° . Let me move del to this position:

Execute Command: `umv del 20.3297`

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "1404.PSIC> umv del 20.3297",  
    "",  
    "      del ",  
    " 20.39371 ",  
    " 20.31018 ",  
    " 20.32971 ",  
    " 20.32971 ",  
    " 20.32971 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 3794901,  
  "last_modified_timestamp": 1749650436.330407,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good, del is now at 20.32971°. Now I need to do at least one more round of optimization. Let me start with a finer eta scan around the current position:

Execute Command: dscan eta -0.2 0.2 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

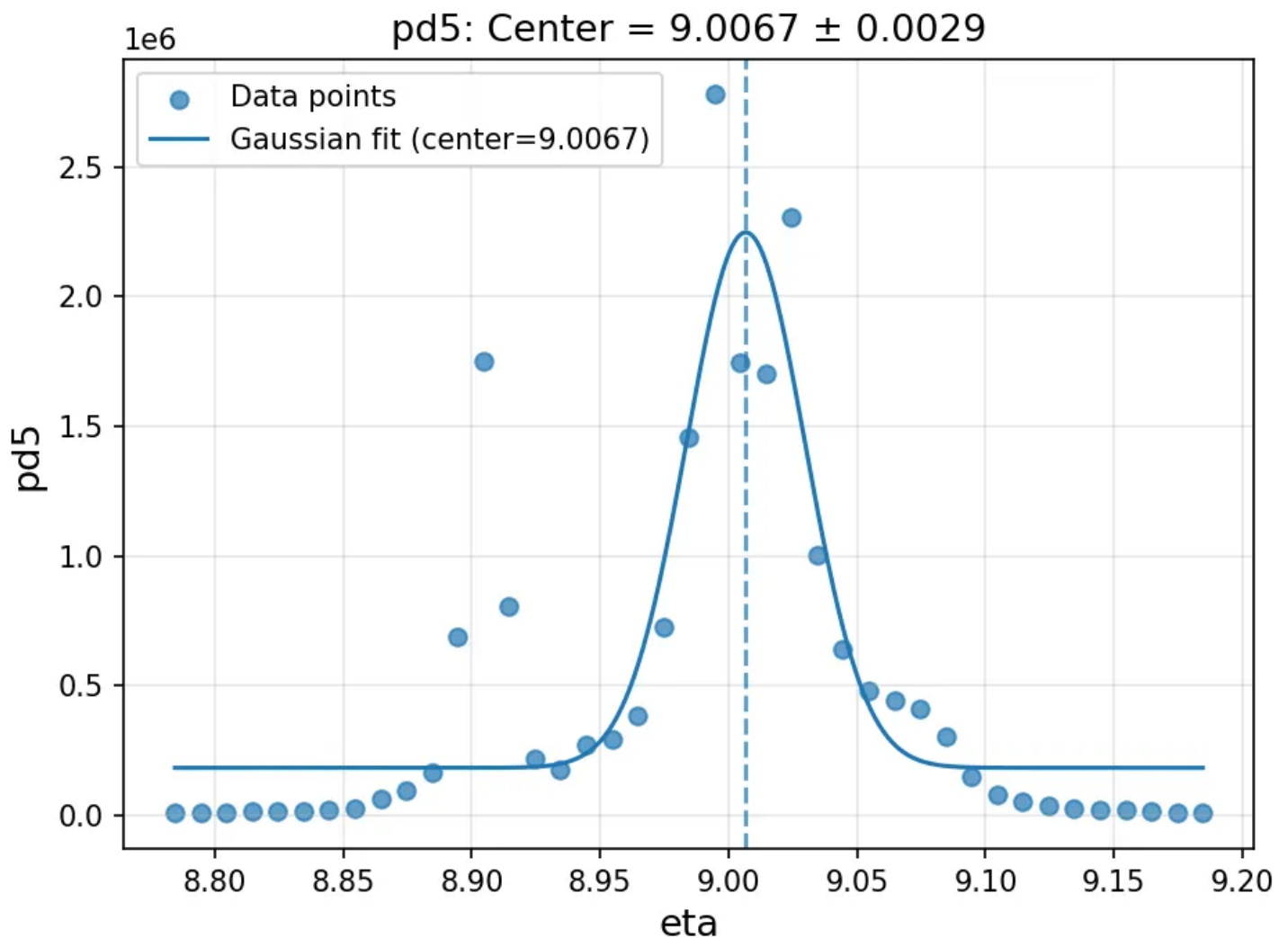
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 39, 9.17449, 0.5000, 0.79006, 0.00041, 0.00555, 0.0048, 0,  
    \"Shutter open.\",  
    \"Shutter closed.\",  
    " 40 9.1845 0.5 0.5 0.5 0.7886 0.00046 0.00546 0.00483  
    \"9.1844922 -0.006910638 -0.00018986309 5.9908286 21177.130 0.7886 0.00046 0.00546 0  
    \" 40, 9.18449, 0.5000, 0.7886, 0.00046, 0.00546, 0.00483, 0,  
    \"/home/det/p2_det/images/mpy_spec_scan73*\",  
    \"\",  
    \"Returning eta to 8.98449\",  
    \"\",  
  ],  
  "file_size_bytes": 3838676,  
  "last_modified_timestamp": 1749650606.196117,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

The eta scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "gaussian",  
  "x_column": "eta",  
  "y_columns": "pd5",  
  "scan_number": "73",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



Good! The peak is now centered at $\eta = 9.0067^\circ$. I notice this peak has a fairly broad profile with some asymmetry. Let me move η to this position:

Execute Command: `umv eta 9.0067`

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "",  
    "1406.PSIC> umv eta 9.0067",  
    "",  
    "      eta ",  
    "  8.99785 ",  
    "  9.00670 ",  
    "  9.00670 ",  
    "  9.00670 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 3838766,  
  "last_modified_timestamp": 1749650640.2076595,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good, eta is now at 9.00670°. Let me do a finer chi scan:

Execute Command: dscan chi -0.2 0.2 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

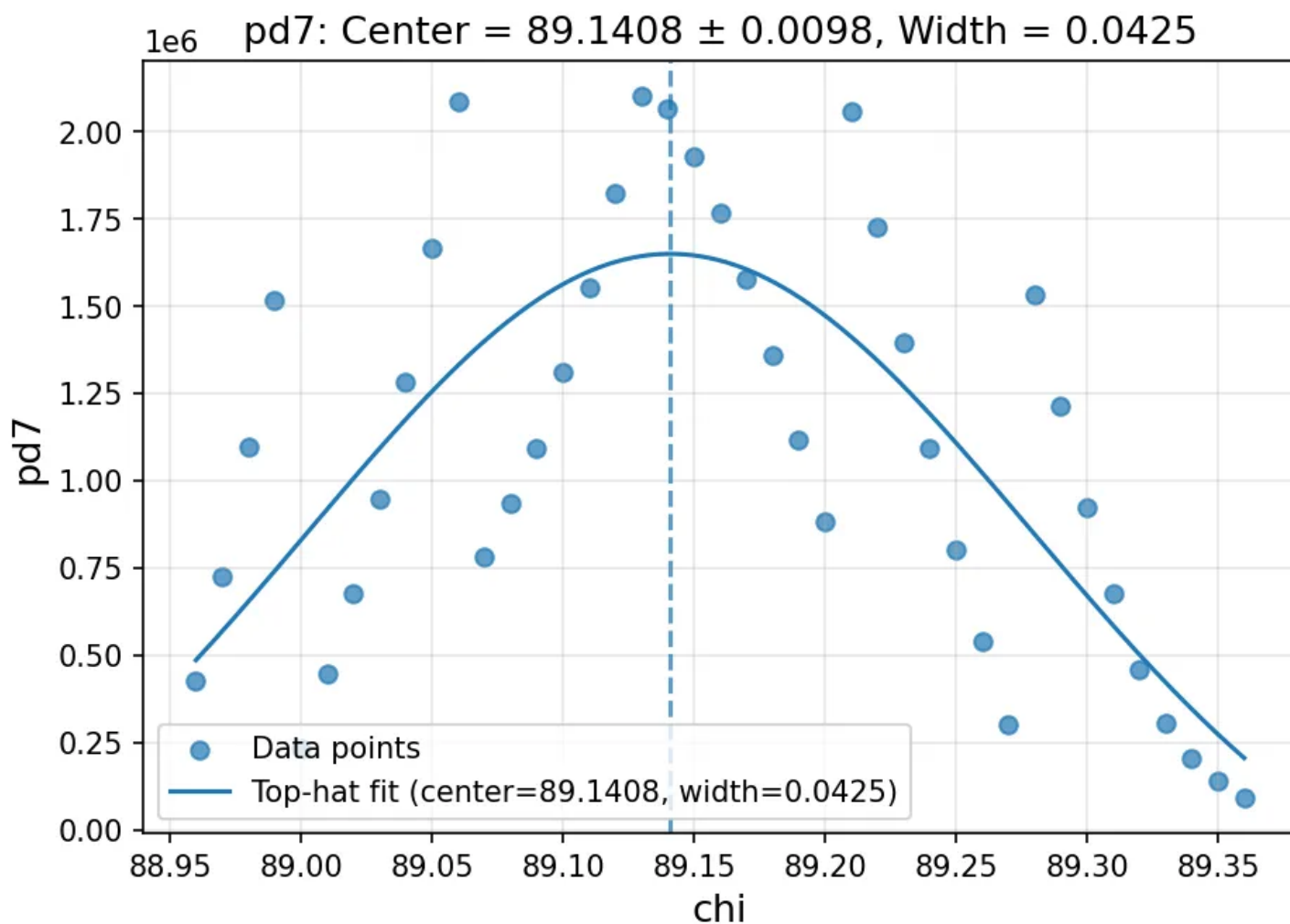
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 39, 89.3498, 0.5000, 0.78992, 0.00041, 0.0054, 0.00483, 0,  
    \"Shutter open.\",  
    \"Shutter closed.\",  
    " 40 89.3598 0.5 0.5 0.5 0.7926 0.00043 0.00542 0.00483  
    \"89.359805 0.0040562454 -0.0083564936 5.9908264 21278.166 0.79256 0.00043 0.00542 0  
    " 40, 89.3598, 0.5000, 0.79256, 0.00043, 0.00542, 0.00483, 0,  
    \"/home/det/p2_det/images/mpy_spec_scan74*\",  
    \"\",  
    \"Returning chi to 89.1598\",  
    \"\",  
  ],  
  "file_size_bytes": 3882991,  
  "last_modified_timestamp": 1749650707.2667294,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
```

The chi scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "tophat",  
  "x_column": "chi",  
  "y_columns": "pd7",  
  "scan_number": "74",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



The peak is centered at $\text{chi} = 89.1408^\circ$. The data shows quite a bit of scatter, which is typical for chi scans. Let me move chi to this position:

Execute Command: umv chi 89.1408

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "1408.PSIC> umv chi 89.1408",  
    "",  
    "      chi ",  
    " 89.14656 ",  
    " 89.12127 ",  
    " 89.14080 ",  
    " 89.14080 ",  
    " 89.14080 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 3883094,  
  "last_modified_timestamp": 1749650776.2898307,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good, chi is now at 89.14080°. Now let me do a finer del scan:

Execute Command: dscan del -0.2 0.2 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

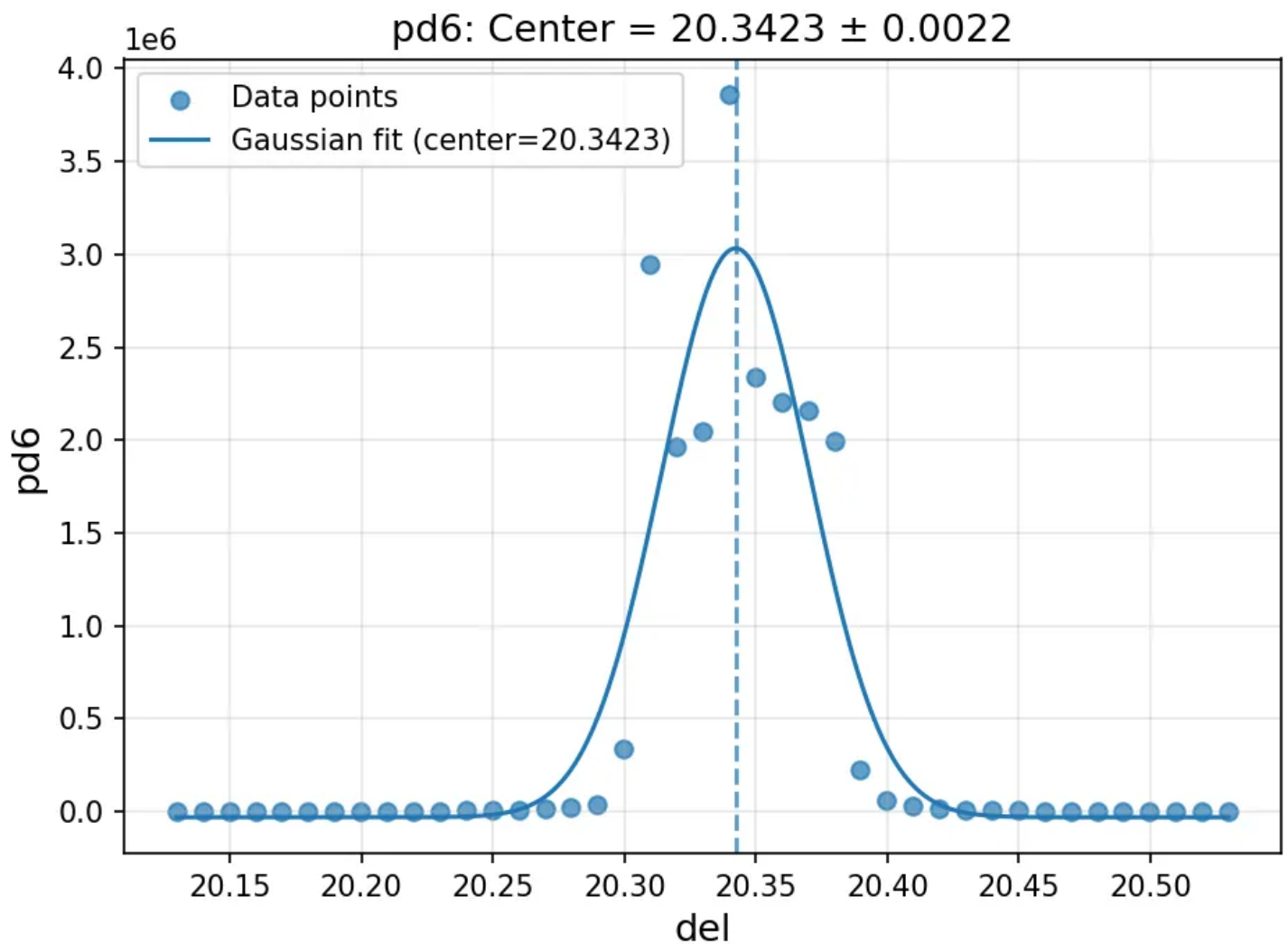
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 39, 20.5197, 0.5000, 0.79034, 0.00039, 0.00541, 0.00486, 0,  
    \"Shutter open.\",  
    \"Shutter closed.\",  
    " 40 20.5297 0.5 0.5 0.5 0.7934 0.00041 0.00549 0.00486  
    \"20.529707 0.0026485317 0.0011625873 6.0491621 21415.883 0.79338 0.00041 0.00549 0.  
    \" 40, 20.5297, 0.5000, 0.79338, 0.00041, 0.00549, 0.00486, 0,  
    \"/home/det/p2_det/images/mpy_spec_scan75*\",  
    \"\",  
    \"Returning del to 20.3297\",  
    \"\",  
  ],  
  "file_size_bytes": 3927117,  
  "last_modified_timestamp": 1749650844.3499165,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
```

The del scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "gaussian",  
  "x_column": "del",  
  "y_columns": "pd6",  
  "scan_number": "75",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



Good! The peak is centered at $\text{del} = 20.3423^\circ$. Let me move del to this position:

Execute Command: umv del 20.3423

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "",  
    "1410.PSIC> umv del 20.3423",  
    "",  
    "    del ",  
    " 20.33641 ",  
    " 20.34230 ",  
    " 20.34230 ",  
    " 20.34230 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 3927208,  
  "last_modified_timestamp": 1749650898.3687782,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good. Now I'll do one final eta scan to ensure optimal positioning:

Execute Command: dscan eta -0.1 0.1 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

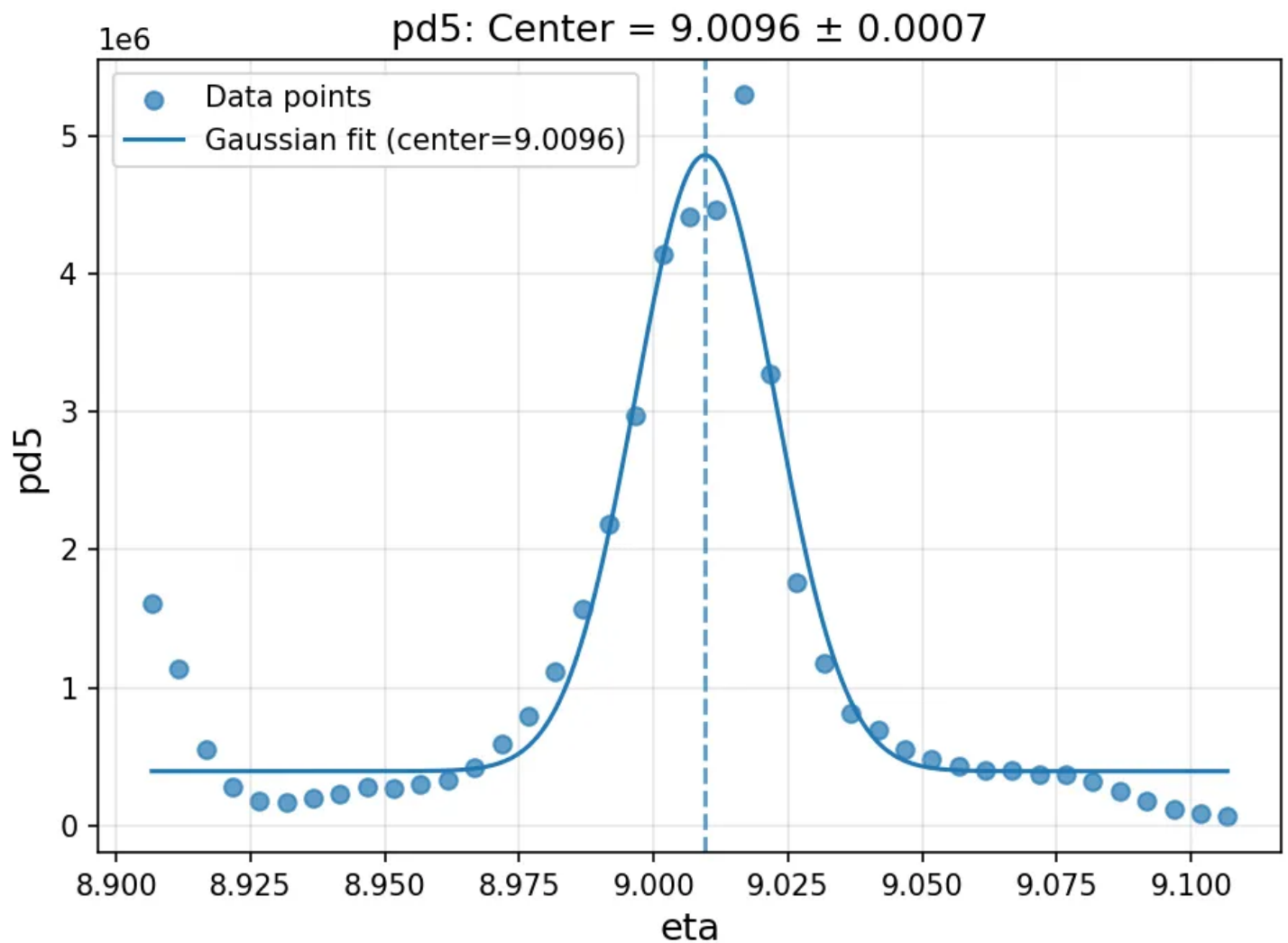
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 39,   9.1017,   0.5000,   0.78906,   0.00038,   0.00546,   0.00483,       0,  
    "Shutter open.",  
    "Shutter closed.",  
    " 40   9.1067      0.5      0.5      0.5   0.7884   0.00044   0.00548   0.0048  
    "9.1066992 -0.0043312014 0.00078034835 5.9945241 21536.894 0.7884 0.00044 0.00548 0  
    " 40,   9.1067,   0.5000,   0.7884,   0.00044,   0.00548,   0.0048,       0,  
    "/home/det/p2_det/images/mpy_spec_scan76*",  
    "",  
    "Returning eta to 9.0067",  
    ""  
  ],  
  "file_size_bytes": 3971252,  
  "last_modified_timestamp": 1749650965.4348502,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

The final eta scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "gaussian",  
  "x_column": "eta",  
  "y_columns": "pd5",  
  "scan_number": "76",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



Excellent! The peak is well-centered at $\eta = 9.0096^\circ$. This is very close to the current position. Let me move eta to this final optimized position:

Execute Command: umv eta 9.0096

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "",  
    "1412.PSIC> umv eta 9.0096",  
    "",  
    "    eta ",  
    "  9.00961 ",  
    "  9.00961 ",  
    "  9.00961 ",  
    "  9.00961 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 3971342,  
  "last_modified_timestamp": 1749651013.450618,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good! Now let me take a final detector image to verify the peak is well-centered:

Execute Command: pd exposure 006_final_optimized 1.0

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "ROI_7_X1=277; ROI_7_Y1=7; ROI_7_X2=279; ROI_7_Y2=187;",  
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",  
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",  
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",  
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",  
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",  
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",  
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",  
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",  
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;"  
  ],  
  "file_size_bytes": 3973286,  
  "last_modified_timestamp": 1749651057.464322,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Let me visualize the final detector image:

read_and_plot_image

Request

```
{
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\006_final_o
}
```

Response

```
{
  "status": "error",
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\006_final_o
  "error": "Image file not found: X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\im
  "error_type": "FileNotFoundError",
  "message": "Failed to read and plot image: Image file not found: X:\\bl17-2\\2025_06_
}
```

Let me check for the most recent image:

explore_directory

Request

```
{
  "max_depth": 1,
  "file_pattern": "006_final_optimized*.raw",
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"
}
```

Response

Directory scan for: X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images
Scan time: 2025-06-11 07:11:20

 images

===== RECENT FILES =====

Let me check all recent files:

explore_directory

Request

```
{  
  "max_depth": 1,  
  "show_recent": true,  
  "file_pattern": "*.raw",  
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"  
}
```

Response

Directory scan for: X:\bl17-2\2025_06_Chen\project_roots\Co3Sn2S2\images
Scan time: 2025-06-11 07:11:25

 images

-  003_initial_061125-032459.raw (1.1 MB), modified 3 hours ago
-  006_eta_centered_061125-044426.raw (1.1 MB), modified 2 hours ago
-  006_eta_centered_061125-063210.raw (1.1 MB), modified 24 minutes ago
-  006_eta_optimized_061125-025321.raw (1.1 MB), modified 4 hours ago
-  006_final_061125-040903.raw (1.1 MB), modified 2 hours ago
-  006_final_optimized_061125-031948.raw (1.1 MB), modified 3 hours ago
-  006_final_optimized_061125-050052.raw (1.1 MB), modified 1 hour ago
-  006_final_optimized_061125-060916.raw (1.1 MB), modified 47 minutes ago
-  006_final_optimized_061125-064812.raw (1.1 MB), modified 8 minutes ago
-  006_initial_061125-024503.raw (1.1 MB), modified 4 hours ago
-  006_initial_061125-034550.raw (1.1 MB), modified 3 hours ago
-  006_initial_061125-044109.raw (1.1 MB), modified 2 hours ago
-  0114_initial_061125-041319.raw (1.1 MB), modified 2 hours ago
-  011_initial_061125-033022.raw (1.1 MB), modified 3 hours ago
-  1010_final_optimized_061125-052442.raw (1.1 MB), modified 1 hour ago
-  1010_initial_061125-051129.raw (1.1 MB), modified 1 hour ago
-  initial_006_search_061125-055400.raw (1.1 MB), modified 1 hour ago
-  initial_check_061125-005204.raw (1.1 MB), modified 6 hours ago
-  optimized_006_061125-010814.raw (1.1 MB), modified 5 hours ago
-  search_006_061125-005441.raw (1.1 MB), modified 6 hours ago
-  search_1014_061125-011920.raw (1.1 MB), modified 5 hours ago
-  test_006_initial_061125-062853.raw (1.1 MB), modified 27 minutes ago

===== RECENT FILES =====

Most recent *.raw files:

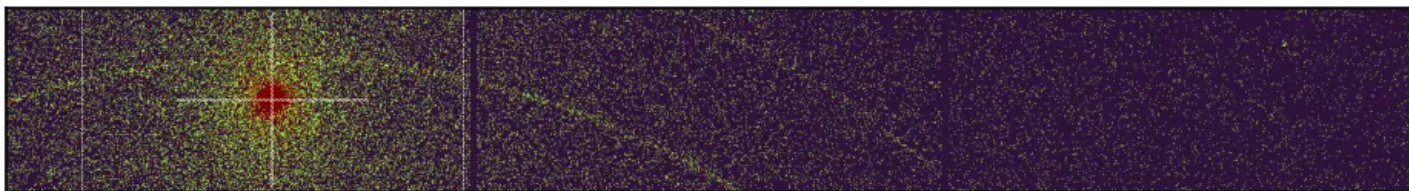
-  006_final_optimized_061125-064812.raw (modified: 2025-06-11 07:03:09)
-  006_eta_centered_061125-063210.raw (modified: 2025-06-11 06:47:07)
-  test_006_initial_061125-062853.raw (modified: 2025-06-11 06:43:49)
-  006_final_optimized_061125-060916.raw (modified: 2025-06-11 06:24:13)
-  initial_006_search_061125-055400.raw (modified: 2025-06-11 06:08:57)

I see the image 006_final_optimized_061125-064812.raw. Let me visualize it:

read_and_plot_image

Request

```
{  
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\006_final_o  
}
```



Perfect! I can see a beautiful, well-centered diffraction peak at the detector center. The peak is bright and clearly visible.

Now I need to check the current 2θ value to optimize the lattice parameter c . Let me check the current position:

Execute Command: wh

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 20  
}
```

Response

```

{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 20,
  "lines_returned": 20,
  "log_lines": [
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;",
    "",
    "1414.PSIC> wh",
    "",
    "H K L = -0.0008447  0.00096668  5.9945\t Lambda = 0.7749 Two Theta = 20.342",
    "",
    "      Alpha      Beta      Psi      Tau      Qaz      Naz      Omega",
    "  32.0105  -32.0044  122.5811  89.9853  90.0000 -173.5784  -1.1615",
    "",
    "      del      eta      chi      phi      nu      mu ",
    "  20.34230    9.00961  89.14080   0.00000   0.00000   0.00000 ",
    ""
  ],
  "file_size_bytes": 3973655,
  "last_modified_timestamp": 1749651111.4821858,
  "message": "Successfully read 20 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}

```

Excellent! The peak is very well centered at H K L = -0.0008447, 0.00096668, 5.9945, which is essentially (0,0,6). The two-theta value is 20.342°.

Now I'll optimize the lattice parameter c based on this measured two-theta value. First, let me get the wavelength:

execute_code

Request

```
{
  "code": "print(f\"Wavelength: {expt.beam.wavelength} Angstroms\")",
  "session_id": "6e65513f-2af4-477e-9e35-fe9ba5ab1bd1"
}
```

Response

Output from session 6e65513f-2af4-477e-9e35-fe9ba5ab1bd1:
Wavelength: 0.7749010390708725 Angstroms

Now I'll optimize the c lattice parameter:

optimize_lattice_parameter

Request

```
{
  "H": 0,
  "K": 0,
  "L": 6,
  "a": 5.3574,
  "b": 5.3574,
  "c": 13.1274,
  "beta": 90,
  "alpha": 90,
  "gamma": 120,
  "store_as": "optimized_lattice",
  "session_id": "6e65513f-2af4-477e-9e35-fe9ba5ab1bd1",
  "wavelength": 0.7749,
  "target_param": "c",
  "two_theta_measured": 20.342
}
```

Response

Lattice Parameter Optimization Results (Session: 6e65513f-2af4-477e-9e35-fe9ba5ab1bd1):

Original Parameters:

$a = 5.357400 \text{ \AA}$, $b = 5.357400 \text{ \AA}$, $c = 13.127400 \text{ \AA}$
 $\alpha = 90.000^\circ$, $\beta = 90.000^\circ$, $\gamma = 120.000^\circ$

Optimized Parameters:

$a = 5.357400 \text{ \AA}$, $b = 5.357400 \text{ \AA}$, $c = 13.164649 \text{ \AA}$
 $\alpha = 90.000^\circ$, $\beta = 90.000^\circ$, $\gamma = 120.000^\circ$

Optimization Details:

Target parameter: c
Original value: 13.127400
Optimized value: 13.164649
Change: 0.037249 (0.28%)

Peak: (0.0, 0.0, 6.0)
Measured 2θ : 20.342°
d-spacing observed: $2.194108 \text{ \AA}$
d-spacing calculated: $2.194108 \text{ \AA}$
d-spacing error: $0.00000020 \text{ \AA}$

Optimization successful: True

Result stored as 'optimized_lattice' in session 6e65513f-2af4-477e-9e35-fe9ba5ab1bd1

Great! The optimized c lattice parameter is $13.1646 \text{ \AA}$ (slightly larger than the initial value of $13.1274 \text{ \AA}$). Now I'll set this as the primary orientation reflection and update the lattice parameters:

Execute Command: setlat 5.3574 5.3574 13.1646 90 90 120

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```

Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    " 32.0105 -32.0044 122.5811 89.9853 90.0000 -173.5784 -1.1615",
    "",
    "      del      eta      chi      phi      nu      mu ",
    " 20.34230    9.00961   89.14080    0.00000    0.00000    0.00000 ",
    "",
    "",
    "1415.PSIC> setlat 5.3574 5.3574 13.1646 90 90 120",
    "#C Wed Jun 11 06:50:28 2025. g_cc reset from 13.163 to 13.1646.",
    "Can't find orientation matrix: Reflections are parallel.",
    ""
  ],
  "file_size_bytes": 3973830,
  "last_modified_timestamp": 1749651191.5054655,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
}
```

Good, the lattice parameters have been updated. The message about parallel reflections is expected since we haven't set the orientation reflections yet. Now let me set this as the primary orientation reflection:

Execute Command: or0 0 0 6

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 20  
}
```

Response

```

{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 20,
  "lines_returned": 20,
  "log_lines": [
    "H K L = -0.0008447  0.00096668  5.9945\\t Lambda = 0.7749 Two Theta = 20.342",
    "",
    "      Alpha      Beta      Psi      Tau      Qaz      Naz      Omega",
    "  32.0105  -32.0044  122.5811  89.9853  90.0000 -173.5784  -1.1615",
    "",
    "      del      eta      chi      phi      nu      mu ",
    "  20.34230    9.00961  89.14080    0.00000    0.00000    0.00000 ",
    "",
    "",
    "1415.PSIC> setlat 5.3574 5.3574 13.1646 90 90 120",
    "#C Wed Jun 11 06:50:28 2025.  g_cc reset from 13.163 to 13.1646.",
    "Can't find orientation matrix: Reflections are parallel.",
    "",
    "",
    "1416.PSIC> or0 0 0 6",
    "#C Wed Jun 11 06:51:01 2025.  g_u00 reset from 20.3446 to 20.3423.",
    "#C Wed Jun 11 06:51:01 2025.  g_u01 reset from 9.43 to 9.00961.",
    "#C Wed Jun 11 06:51:01 2025.  g_u02 reset from 89.2846 to 89.1408.",
    "Can't find orientation matrix: Reflections are parallel.",
    ""
  ],
  "file_size_bytes": 3974109,
  "last_modified_timestamp": 1749651225.5170093,
  "message": "Successfully read 20 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}

```

Good! The primary orientation reflection has been set. The message about parallel reflections is normal since we only have one reflection so far. Now I need to find a second, non-parallel reference reflection.

Let me check the sample information again to find suitable (H,0,L) or (0,K,L) peaks with $\text{theta_minus_rel_angle} > 2$:

call_method

Request

```
{  
  "arguments": "sort_by='theta_minus_rel_angle', ascending=False, max_rows=40",  
  "session_id": "6e65513f-2af4-477e-9e35-fe9ba5ab1bd1",  
  "method_name": "get_sample_information",  
  "object_name": "expt"  
}
```

Response

Result of `expt.get_sample_information()` in session `6e65513f-2af4-477e-9e35-fe9ba5ab1bd1`

Incident X-ray wavelength: 0.7749 Angstrom

Sample Structure Information

```

Structure Summary:  $\text{Co}_3(\text{SnS})_2$

Lattice

abc : 5.3574 5.3574 13.1274

angles : 90.0000 90.0000 120.0000

volume : 326.2991

A : 5.3574 0.0000 0.0000

B : -2.6787 4.6396 0.0000

C : 0.0000 0.0000 13.1274

pbcs : True True True

```

Diffraction Peak Analysis

Diffraction Data Table

Table contains 29 total rows, sorted by ``theta_minus_rel_angle`` in descending order.

#	tth	intensity	d_hkl	theta_minus_rel_angle	hkl indices
---	----	-----	-----	-----	-----
1	52.5551	0.3387	0.8752	26.2775	[0 0 15]
2	41.4859	4.2287	1.0939	20.7429	[0 0 12]
3	30.8090	3.9315	1.4586	15.4045	[0 0 9]
4	49.8661	3.7299	0.9191	13.5075	[0 1 14]
5	49.8661	3.7299	0.9191	13.5075	[1 -1 14]
6	49.8661	3.7299	0.9191	13.5075	[-1 0 14]
7	46.2418	0.0470	0.9867	10.8422	[1 0 13]
8	46.2418	0.0470	0.9867	10.8422	[0 -1 13]
9	46.2418	0.0470	0.9867	10.8422	[-1 1 13]
10	20.4004	37.0756	2.1879	10.2002	[0 0 6]
11	39.1729	1.1225	1.1558	5.1616	[0 1 11]
12	39.1729	1.1225	1.1558	5.1616	[1 -1 11]
13	39.1729	1.1225	1.1558	5.1616	[-1 0 11]
14	10.1597	26.7452	4.3758	5.0798	[0 0 3]
15	52.9341	9.7012	0.8693	4.4585	[2 0 14]
16	52.9341	9.7012	0.8693	4.4585	[-2 2 14]
17	52.9341	9.7012	0.8693	4.4585	[0 -2 14]
18	35.7249	7.1978	1.2632	2.0641	[1 0 10]

19	35.7249	7.1978	1.2632	2.0641	[-1 1 10]
20	35.7249	7.1978	1.2632	2.0641	[0 -1 10]
21	49.4755	1.7922	0.9259	1.2146	[2 -2 13]
22	49.4755	1.7922	0.9259	1.2146	[0 2 13]
23	49.4755	1.7922	0.9259	1.2146	[-2 0 13]
24	44.9862	3.4488	1.0128	0.2785	[2 -1 12]
25	44.9862	3.4488	1.0128	0.2785	[1 1 12]
26	44.9862	3.4488	1.0128	0.2785	[-1 2 12]
27	44.9862	3.4488	1.0128	0.2785	[-1 -1 12]
28	44.9862	3.4488	1.0128	0.2785	[-2 1 12]
29	44.9862	3.4488	1.0128	0.2785	[1 -2 12]

Summary Statistics

Key Values

Statistic	tth	intensity	d_hkl	
:-----	:-----:	:-----:	:-----:	
min	10.1597	0.0470	0.8693	
max	52.9341	37.0756	4.3758	
mean	42.9508	5.6477	1.1872	

Column Descriptions

- ****tth****: Two-theta angle (in degrees)
- ****intensity****: Relative intensity of the diffraction peak
- ****d_hkl****: Interplanar spacing (in Angstroms)
- ****hkl indices****: Miller indices representing structural peaks [h k l]

_Note: This data combines the crystal structure parameters with calculated diffraction

Looking at the table, I need to find peaks with `theta_minus_rel_angle > 2`. The good candidates are:

1. (0,1,11) with `theta_minus_rel_angle = 5.1616` (1.1% intensity)
2. (1,0,10) with `theta_minus_rel_angle = 2.0641` (7.2% intensity)
3. (0,1,14) with `theta_minus_rel_angle = 13.5075` (3.7% intensity)
4. (2,0,14) with `theta_minus_rel_angle = 4.4585` (9.7% intensity)

Let me go with (1,0,10) since it has good intensity (7.2%) and `theta_minus_rel_angle = 2.0641 > 2`.

For vertical geometry, I'll set:

- `eta = theta_minus_rel_angle = 2.0641°`
- `del ≈ 2θ = 35.7249°`

But I need to account for the motor offset I observed earlier (about -1.22° in eta). So I'll use:

- $\text{eta} \approx 2.0641 - 1.22 = 0.84^\circ$

Execute Command: umv eta 0.84 del 35.7249

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 15  
}
```

Response

```

{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",
  "lines_requested": 15,
  "lines_returned": 15,
  "log_lines": [
    "  0.84000  30.43857 ",
    "  0.84000  31.03365 ",
    "  0.84000  31.60980 ",
    "  0.84000  32.18674 ",
    "  0.84000  32.77203 ",
    "  0.84000  33.34861 ",
    "  0.84000  33.94455 ",
    "  0.84000  34.53922 ",
    "  0.84000  35.11627 ",
    "  0.84000  35.65689 ",
    "  0.84000  35.72490 ",
    "  0.84000  35.72490 ",
    "  0.84000  35.72490 ",
    "",
    ""
  ],
  "file_size_bytes": 3974838,
  "last_modified_timestamp": 1749651285.5439692,
  "message": "Successfully read 15 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}

```

Good, the motors have moved. Since I'm looking for a (1,0,10) peak which has an in-plane component, I'll need to scan phi to find it. Let me first take an image to see if there's anything visible:

Execute Command: pd exposure 1010_initial_search 1.0

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "ROI_7_X1=277; ROI_7_Y1=7; ROI_7_X2=279; ROI_7_Y2=187;",  
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",  
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",  
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",  
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",  
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",  
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",  
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",  
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",  
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;"  
  ],  
  "file_size_bytes": 3976743,  
  "last_modified_timestamp": 1749651332.5587208,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"  
}
```

Let me visualize the image:

read_and_plot_image

Request

```
{  
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\1010_initia  
}
```

Response

```
{
  "status": "error",
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\1010_initia
"error": "Image file not found: X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\im
"error_type": "FileNotFoundError",
  "message": "Failed to read and plot image: Image file not found: X:\\bl17-2\\2025_06_
}
```

Let me check for the recent files:

explore_directory

Request

```
{
  "max_depth": 1,
  "file_pattern": "1010_initial*.raw",
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"
}
```

Response

Directory scan for: X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images
Scan time: 2025-06-11 07:16:00

 images

===== RECENT FILES =====

Let me check all recent images:

explore_directory

Request

```
{  
  "max_depth": 1,  
  "show_recent": true,  
  "file_pattern": "*.raw",  
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"  
}
```

Response

Directory scan for: X:\bl17-2\2025_06_Chen\project_roots\Co3Sn2S2\images
Scan time: 2025-06-11 07:16:06

 images

-  003_initial_061125-032459.raw (1.1 MB), modified 3 hours ago
-  006_eta_centered_061125-044426.raw (1.1 MB), modified 2 hours ago
-  006_eta_centered_061125-063210.raw (1.1 MB), modified 28 minutes ago
-  006_eta_optimized_061125-025321.raw (1.1 MB), modified 4 hours ago
-  006_final_061125-040903.raw (1.1 MB), modified 2 hours ago
-  006_final_optimized_061125-031948.raw (1.1 MB), modified 3 hours ago
-  006_final_optimized_061125-050052.raw (1.1 MB), modified 2 hours ago
-  006_final_optimized_061125-060916.raw (1.1 MB), modified 51 minutes ago
-  006_final_optimized_061125-064812.raw (1.1 MB), modified 12 minutes ago
-  006_initial_061125-024503.raw (1.1 MB), modified 4 hours ago
-  006_initial_061125-034550.raw (1.1 MB), modified 3 hours ago
-  006_initial_061125-044109.raw (1.1 MB), modified 2 hours ago
-  0114_initial_061125-041319.raw (1.1 MB), modified 2 hours ago
-  011_initial_061125-033022.raw (1.1 MB), modified 3 hours ago
-  1010_final_optimized_061125-052442.raw (1.1 MB), modified 1 hour ago
-  1010_initial_061125-051129.raw (1.1 MB), modified 1 hour ago
-  1010_initial_search_061125-065247.raw (1.1 MB), modified 8 minutes ago
-  initial_006_search_061125-055400.raw (1.1 MB), modified 1 hour ago
-  initial_check_061125-005204.raw (1.1 MB), modified 6 hours ago
-  optimized_006_061125-010814.raw (1.1 MB), modified 5 hours ago
-  search_006_061125-005441.raw (1.1 MB), modified 6 hours ago
-  search_1014_061125-011920.raw (1.1 MB), modified 5 hours ago
-  test_006_initial_061125-062853.raw (1.1 MB), modified 32 minutes ago

===== RECENT FILES =====

Most recent *.raw files:

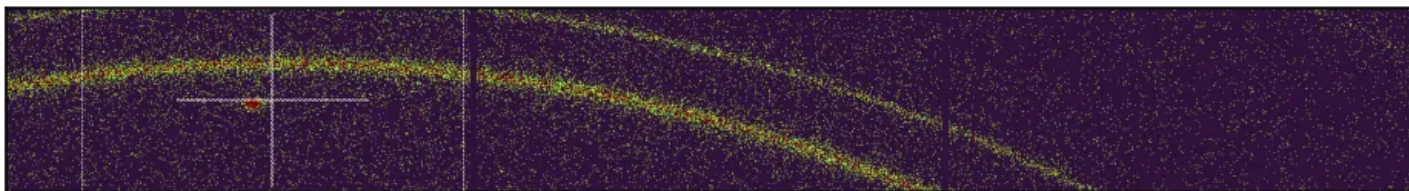
-  1010_initial_search_061125-065247.raw (modified: 2025-06-11 07:07:43)
-  006_final_optimized_061125-064812.raw (modified: 2025-06-11 07:03:09)
-  006_eta_centered_061125-063210.raw (modified: 2025-06-11 06:47:07)
-  test_006_initial_061125-062853.raw (modified: 2025-06-11 06:43:49)
-  006_final_optimized_061125-060916.raw (modified: 2025-06-11 06:24:13)

I see the file 1010_initial_search_061125-065247.raw. Let me visualize it:

read_and_plot_image

Request

```
{
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\1010_initia
}
```



I can see a powder ring pattern, which indicates I need to find the right phi angle. The hexagonal crystal has 6-fold symmetry, so I should expect peaks every 60° in phi. Let me do a wide phi scan to find the peak positions:

Execute Command: dscan phi -30 30 60 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```

Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    " 59,          29,    0.5000,  0.79166,  0.00042,  0.00613,  0.00483,          0,
    \"Shutter open.\",
    \"Shutter closed.\",
    \" 60   30.0000      0.5      0.5      0.5   0.7932  0.00044  0.00614  0.00483
    \"30 0.47953764 0.656923 10.028512 22040.937 0.79319 0.00044 0.00614 0.00483 0 0 0 1
    \" 60,          30,    0.5000,  0.79319,  0.00044,  0.00614,  0.00483,          0,
    \"/home/det/p2_det/images/mpy_spec_scan77*\",
    \"\",
    \"Returning phi to 0\",
    \"\",
  ],
  "file_size_bytes": 4037936,
  "last_modified_timestamp": 1749651473.6699772,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```

Good, the scan is complete. Let me visualize it to find the peaks:

read_and_plot_spec

Request

```
{
  "fit_type": "tophat",
  "x_column": "phi",
  "y_columns": "pd5",
  "scan_number": "77",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"
}
```

Response

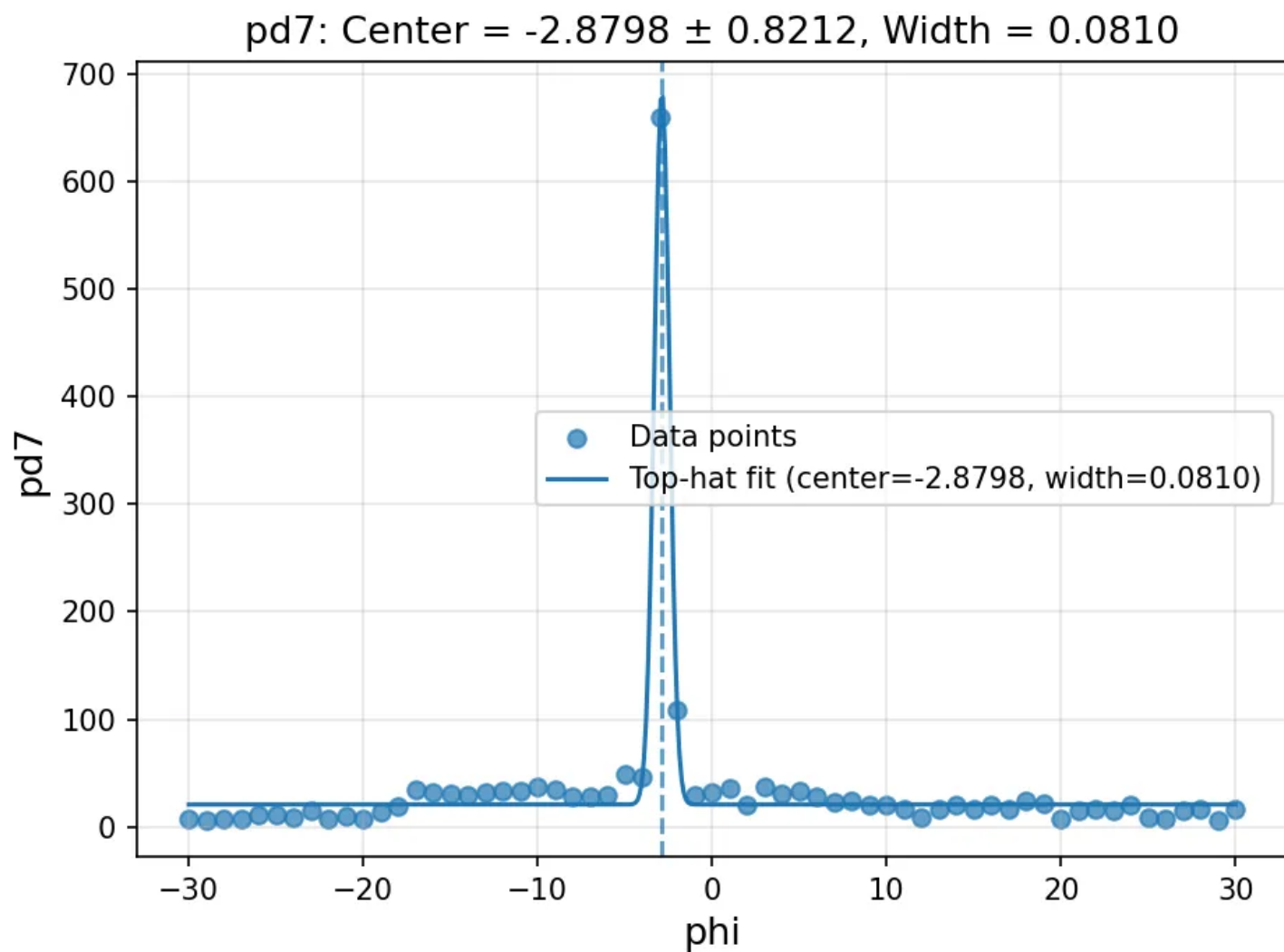
```
{
  "status": "error",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec",
  "scan_number": "77",
  "error": "Invalid y_column for phi. For phi, y_column must be 'pd7'.",
  "error_type": "ValueError",
  "message": "Failed to read and plot SPEC data: Invalid y_column for phi. For phi, y_c
}
```

Let me use pd7 for the phi scan:

read_and_plot_spec

Request

```
{
  "fit_type": "tophat",
  "x_column": "phi",
  "y_columns": "pd7",
  "scan_number": "77",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"
}
```



Excellent! I found a sharp peak at $\phi = -2.8798^\circ$. Let me move ϕ to this position:

Execute Command: `umv phi -2.8798`

Prompt:

Please read the log and continue.

Response:

`read_log`

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "    phi ",  
    " -0.02676 ",  
    " -1.56402 ",  
    " -2.91883 ",  
    " -2.91887 ",  
    " -2.87980 ",  
    " -2.87980 ",  
    " -2.87980 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 4038063,  
  "last_modified_timestamp": 1749651524.686793,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good, phi is now at -2.8798°. Now I need to perform eta scan to locate the peak precisely:

Execute Command: dscan eta -1 1 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```

Response

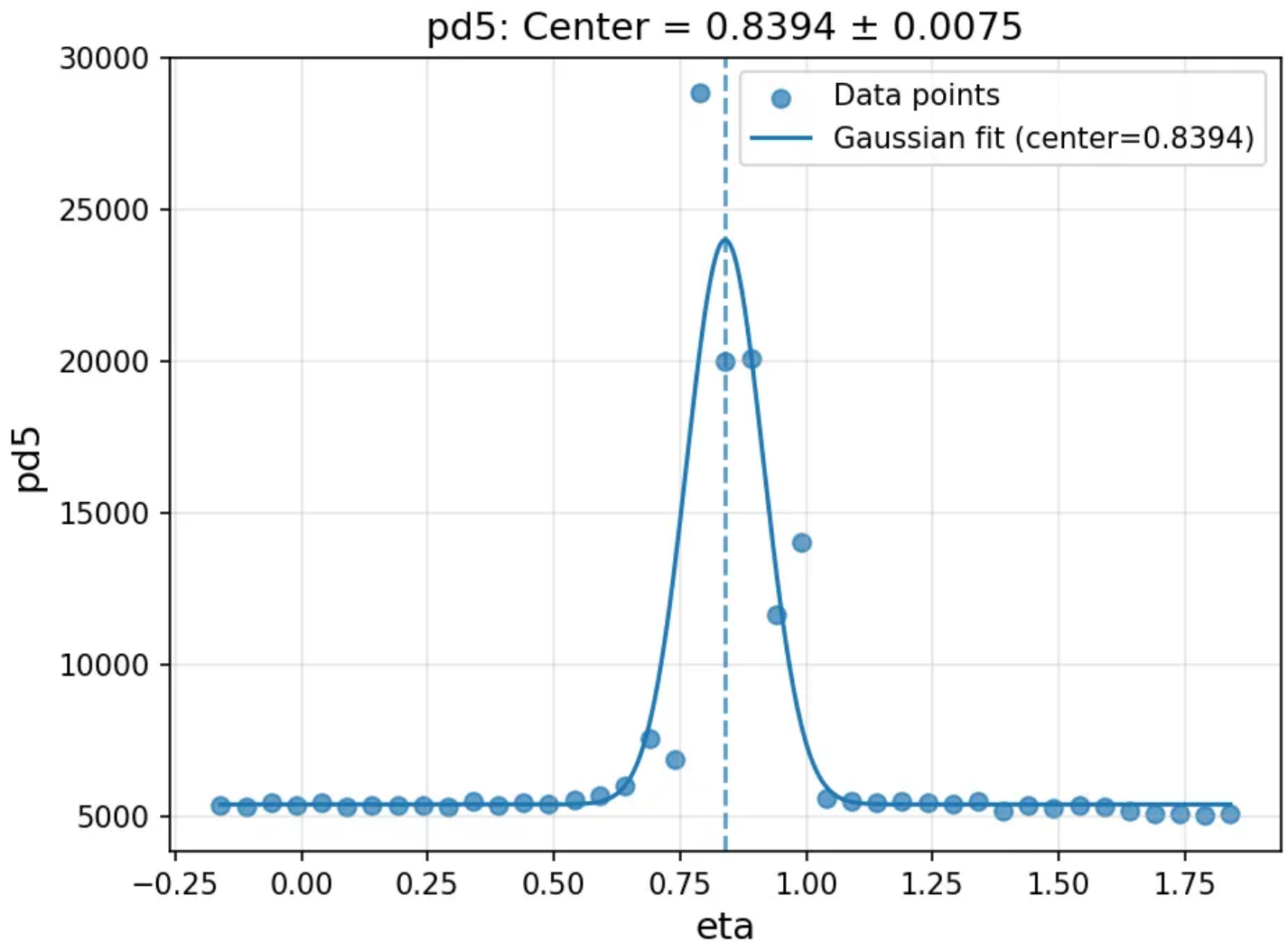
```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    " 39,      1.79,    0.5000,  0.79075,  0.00039,  0.00578,  0.00486,      0,
    "Shutter open.",
    "Shutter closed.",
    " 40    1.8400      0.5      0.5      0.5  0.7893  0.00037  0.0056  0.00483
    "1.84 0.9482424 -0.008145023 10.062518 22161.847 0.78928 0.00037 0.0056 0.00483 0 0
    " 40,      1.84,    0.5000,  0.78928,  0.00037,  0.0056,  0.00483,      0,
    "/home/det/p2_det/images/mpy_spec_scan78*",
    "",
    "Returning eta to 0.84",
    ""
  ],
  "file_size_bytes": 4080550,
  "last_modified_timestamp": 1749651590.7468493,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
}
```

The eta scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{
  "fit_type": "gaussian",
  "x_column": "eta",
  "y_columns": "pd5",
  "scan_number": "78",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"
}
```



Perfect! I found a strong peak centered at $\eta = 0.8394^\circ$. This confirms the η offset is about -1.22° as I estimated. Let me move η to this position:

Execute Command: `umv eta 0.8394`

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "1422.PSIC> umv eta .8394",  
    "",  
    "      eta ",  
    "  0.82668 ",  
    "  0.80033 ",  
    "  0.83939 ",  
    "  0.83939 ",  
    "  0.83939 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 4080651,  
  "last_modified_timestamp": 1749651640.7646492,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good, eta is now at 0.83939°. Now I need to perform a fine eta scan to get better precision:

Execute Command: dscan eta -0.1 0.1 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

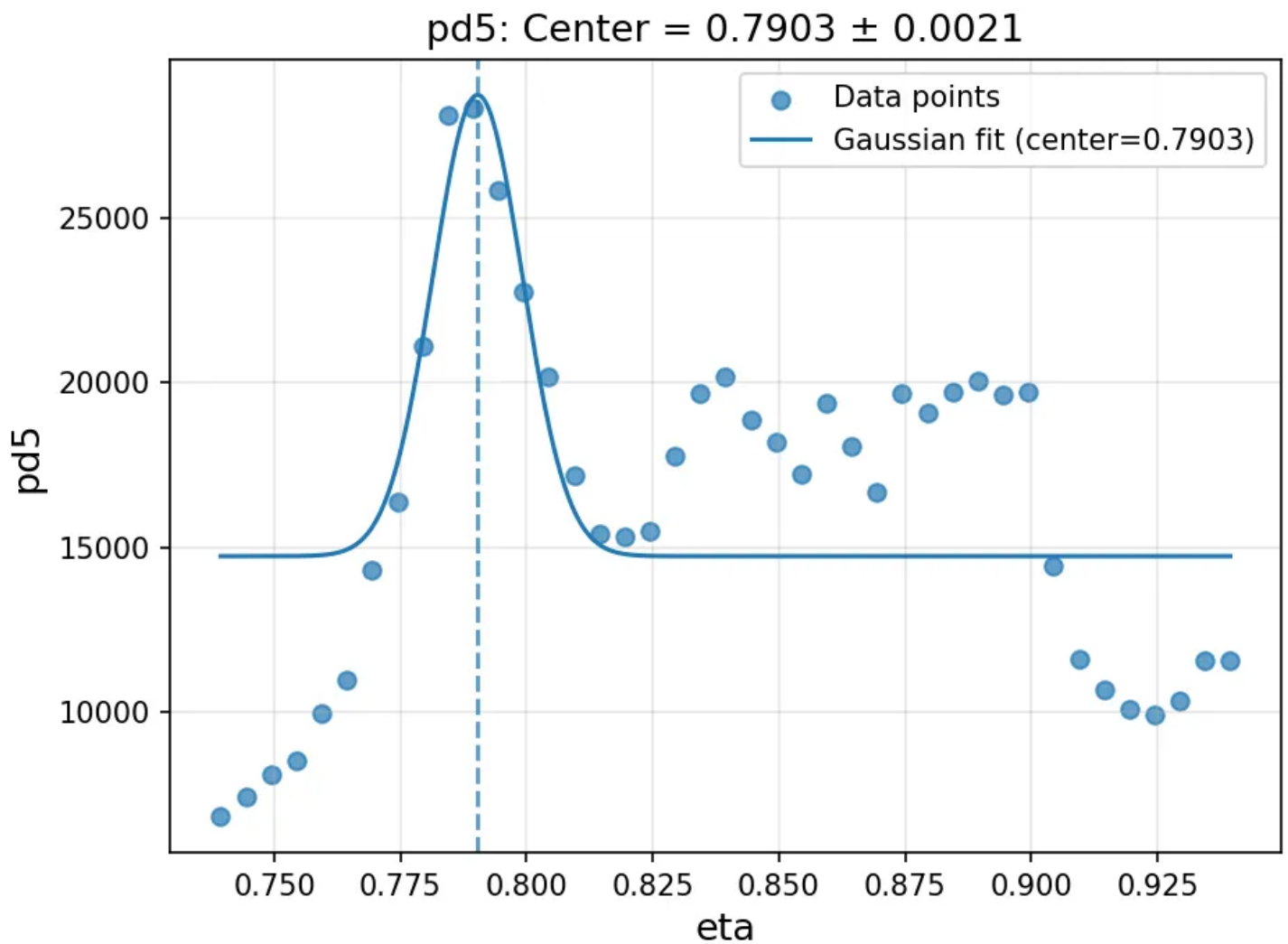
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 39, 0.934395, 0.5000, 0.79708, 0.0003, 0.00578, 0.00486, 0,  
    "Shutter open.",  
    "Shutter closed.",  
    " 40 0.9394 0.5 0.5 0.5 0.795 0.00037 0.00577 0.00486  
    "0.93939453 1.0040795 -0.0084685683 10.019204 22275.089 0.795 0.00037 0.00577 0.004  
    " 40, 0.939395, 0.5000, 0.795, 0.00037, 0.00577, 0.00486, 0,  
    "/home/det/p2_det/images/mpy_spec_scan79*",  
    "",  
    "Returning eta to 0.839395",  
    ""  
  ],  
  "file_size_bytes": 4123774,  
  "last_modified_timestamp": 1749651703.8206575,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

The fine eta scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "gaussian",  
  "x_column": "eta",  
  "y_columns": "pd5",  
  "scan_number": "79",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



Good! The peak is centered at $\eta = 0.7903^\circ$. The data shows some noise but the main peak is clear.
Let me move eta to this position:

Execute Command: umv eta 0.7903

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "1424.PSIC> umv eta .7903",  
    "",  
    "      eta ",  
    "  0.82582 ",  
    "  0.75123 ",  
    "  0.79029 ",  
    "  0.79029 ",  
    "  0.79029 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 4123875,  
  "last_modified_timestamp": 1749651743.8342972,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good, eta is now at 0.79029°. Now I need to scan chi to center the peak horizontally:

Execute Command: dscan chi -1 1 20 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

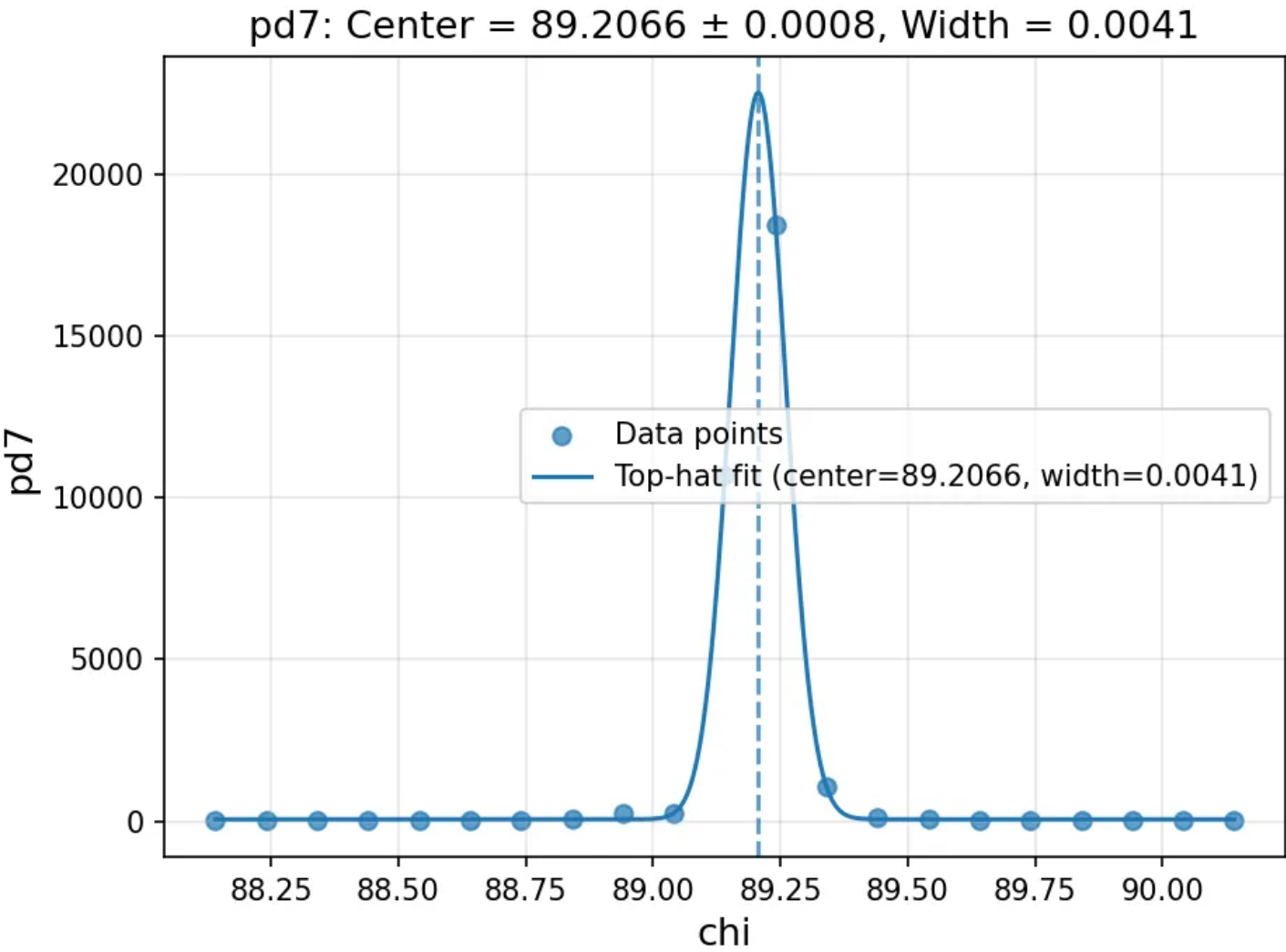
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "  19,  90.0408,   0.5000,  0.79356,  0.00038,  0.00564,  0.00483,      0,  
    \"Shutter open.\",  
    \"Shutter closed.\",  
    " 20  90.1408      0.5      0.5      0.5  0.7927  0.00037  0.00565  0.00483  
    \"90.140801 1.048371 -0.079279636 10.010174 22369.885 0.79269 0.00037 0.00565 0.0048  
    "  20,  90.1408,   0.5000,  0.79269,  0.00037,  0.00565,  0.00483,      0,  
    \"/home/det/p2_det/images/mpy_spec_scan80*\",  
    \"\",  
    \"Returning chi to 89.1408\",  
    \"\",  
  ],  
  "file_size_bytes": 4147460,  
  "last_modified_timestamp": 1749651798.8801775,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
```

The chi scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{
  "fit_type": "tophat",
  "x_column": "chi",
  "y_columns": "pd7",
  "scan_number": "80",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"
}
```



Excellent! I found a very sharp peak at $\text{chi} = 89.2066^\circ$. The fitted width is extremely narrow (0.0041°), which indicates I need to do a finer scan. Let me move chi to this position first:

Execute Command: umv chi 89.2066

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "",  
    "1426.PSIC> umv chi 89.2066",  
    "",  
    "      chi ",  
    " 89.15412 ",  
    " 89.20660 ",  
    " 89.20660 ",  
    " 89.20660 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 4147551,  
  "last_modified_timestamp": 1749651849.895993,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good. Now let me do a finer chi scan around this position since the peak is very sharp (FWHM $\approx$ 0.0041°). I'll scan $\pm 0.02^\circ$ with smaller steps:

Execute Command: dscan chi -0.02 0.02 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

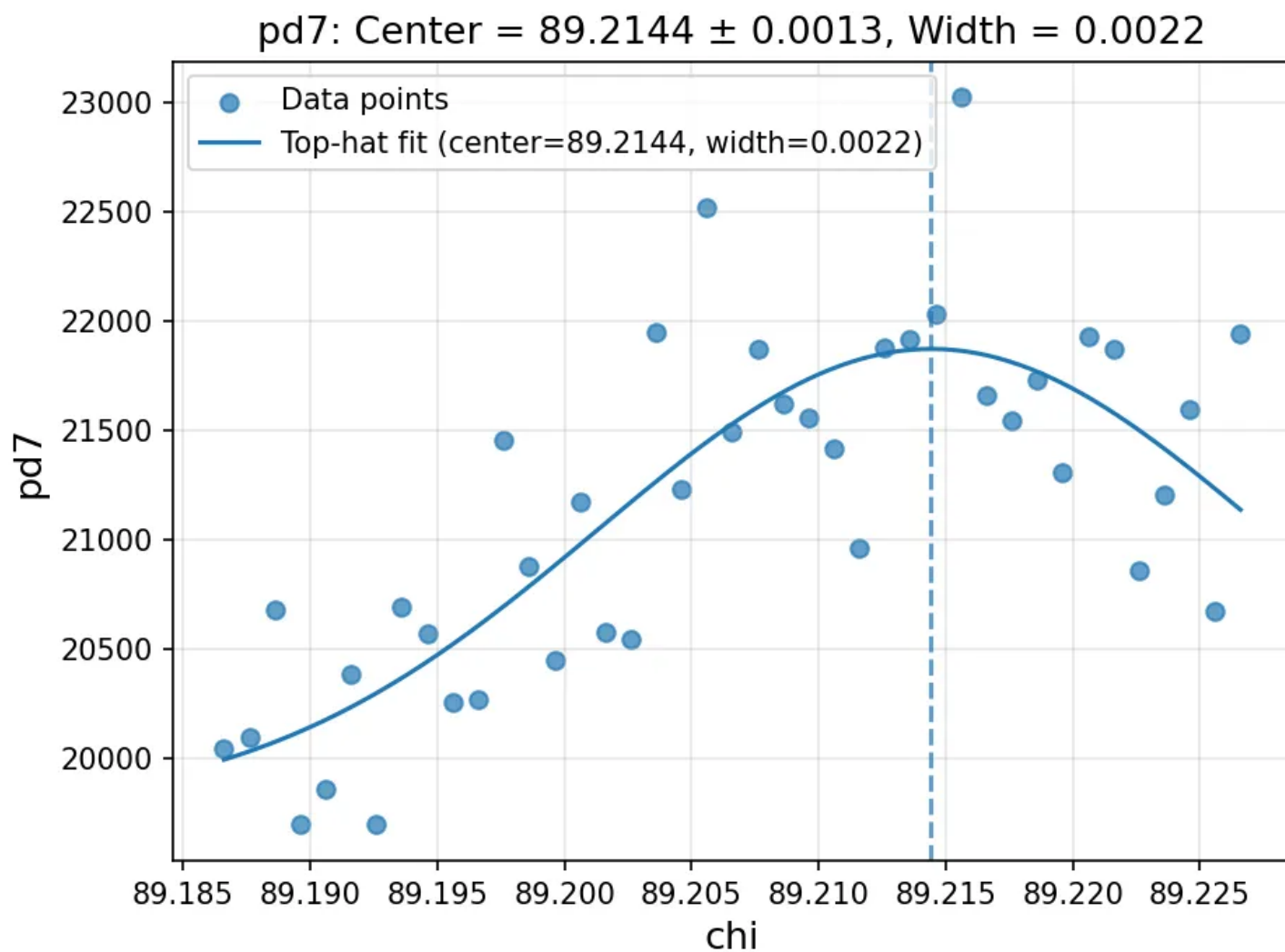
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 39, 89.2256, 0.5000, 0.80086, 0.00042, 0.00567, 0.00486, 0,  
    \"Shutter open.\",  
    \"Shutter closed.\",  
    " 40 89.2266 0.5 0.5 0.5 0.7995 0.00049 0.00561 0.00486  
    \"89.226602 1.0163086 -0.01459333 10.011774 22492.885 0.79947 0.00049 0.00561 0.0048  
    " 40, 89.2266, 0.5000, 0.79947, 0.00049, 0.00561, 0.00486, 0,  
    \"/home/det/p2_det/images/mpy_spec_scan81*\",  
    \"\",  
    \"Returning chi to 89.2066\",  
    \"\",  
  ],  
  "file_size_bytes": 4190661,  
  "last_modified_timestamp": 1749651921.987146,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
```

The fine chi scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "tophat",  
  "x_column": "chi",  
  "y_columns": "pd7",  
  "scan_number": "81",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



Good! The finer scan shows the peak is centered at $\text{chi} = 89.2144^\circ$. Let me move chi to this position:

Execute Command: umv chi 89.2144

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "",  
    "1428.PSIC> umv chi 89.2144",  
    "",  
    "      chi ",  
    " 89.21432 ",  
    " 89.21439 ",  
    " 89.21439 ",  
    " 89.21439 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 4190752,  
  "last_modified_timestamp": 1749651976.0050097,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good. Now let me scan del to center the peak vertically:

Execute Command: dscan del -1 1 20 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

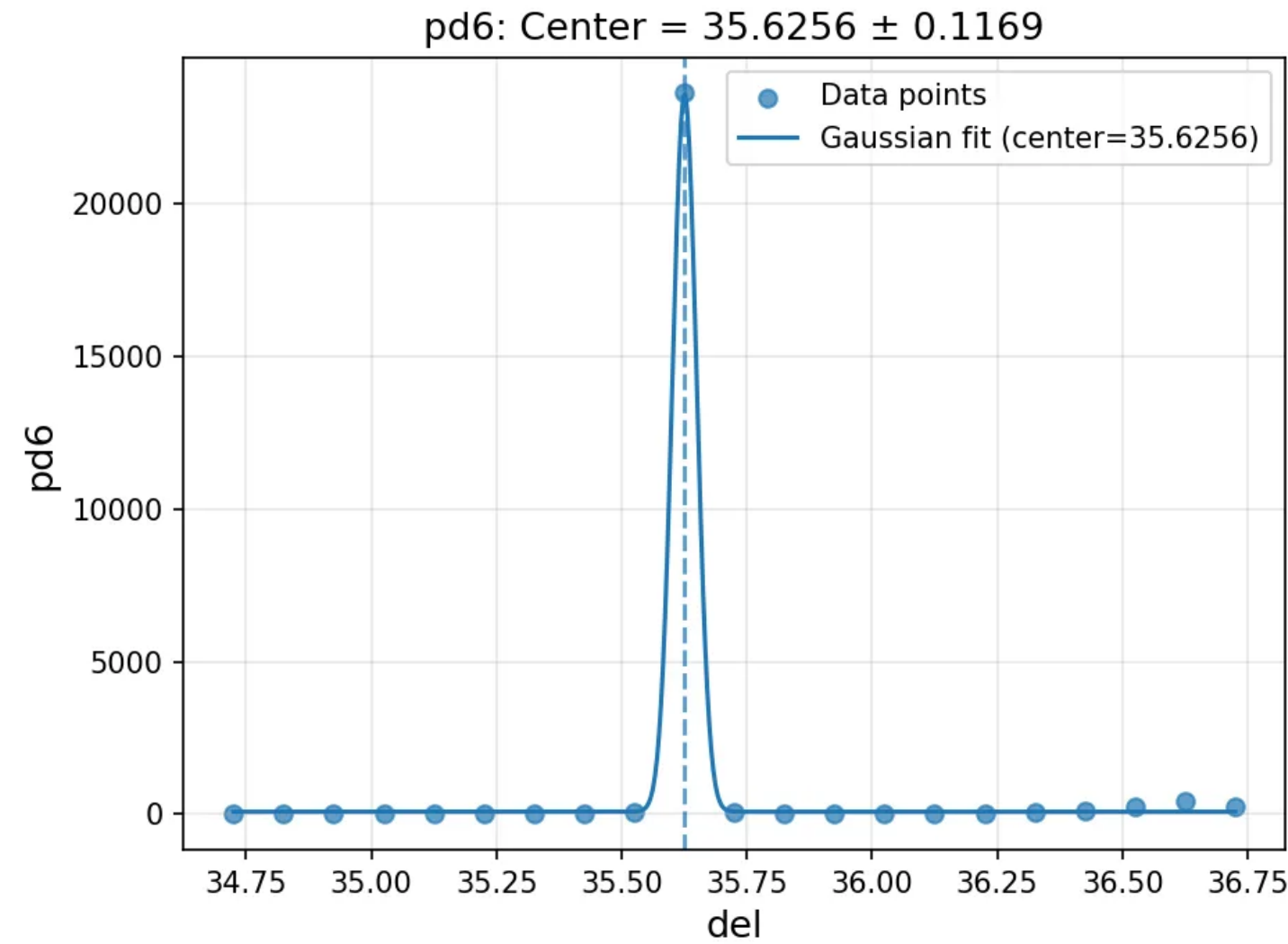
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 19, 36.6249, 0.5000, 0.7944, 0.00042, 0.00577, 0.0048, 0,  
    \"Shutter open.\",  
    \"Shutter closed.\",  
    " 20 36.7249 0.5 0.5 0.5 0.7944 0.00038 0.00576 0.0048  
    \"36.724902 1.0750483 -0.014269619 10.256473 22604.048 0.79443 0.00038 0.00576 0.004  
    " 20, 36.7249, 0.5000, 0.79443, 0.00038, 0.00576, 0.0048, 0,  
    \"/home/det/p2_det/images/mpy_spec_scan82*\",  
    \"\",  
    \"Returning del to 35.7249\",  
    \"\",  
  ],  
  "file_size_bytes": 4214375,  
  "last_modified_timestamp": 1749652033.0509217,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
```

The del scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{
  "fit_type": "gaussian",
  "x_column": "del",
  "y_columns": "pd6",
  "scan_number": "82",
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"
}
```



Good! The peak is centered at del = 35.6256°. Let me move del to this position:

Execute Command: umv del 35.6256

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "1430.PSIC> umv del 35.6256",  
    "",  
    "      del ",  
    " 35.71820 ",  
    " 35.60607 ",  
    " 35.62561 ",  
    " 35.62561 ",  
    " 35.62561 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 4214478,  
  "last_modified_timestamp": 1749652083.0677216,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good. Now I need to do at least one more round of optimization. Let me start with another eta scan:

Execute Command: dscan eta -0.1 0.1 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```

Response

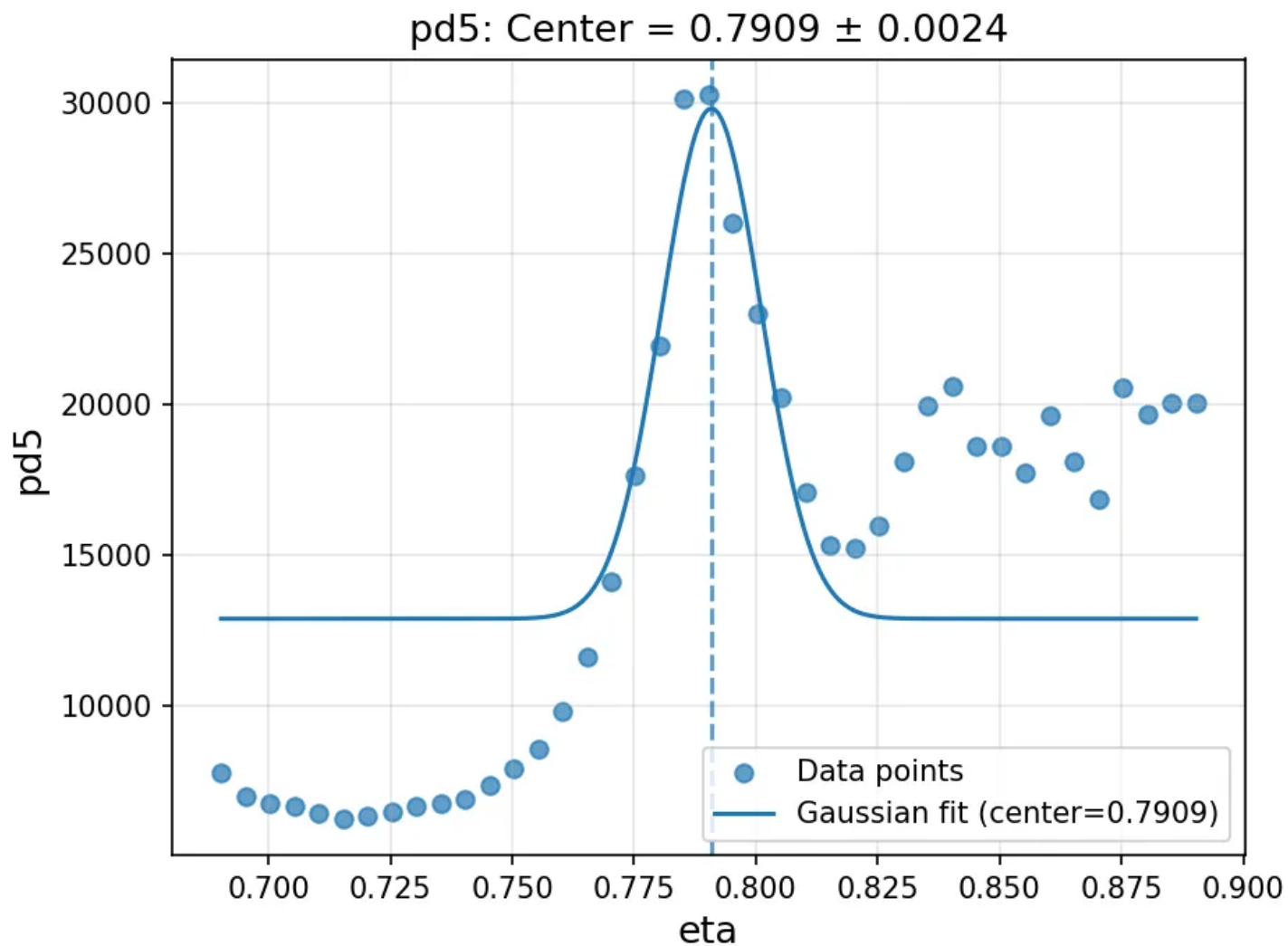
```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    " 39, 0.885293, 0.5000, 0.79248, 0.00042, 0.00584, 0.00486, 0,
    \"Shutter open.\",
    \"Shutter closed.\",
    \" 40 0.8903 0.5 0.5 0.5 0.7887 0.00038 0.00576 0.00483
    \"0.89029297 1.0039211 -0.013643352 9.9922716 22716.074 0.78871 0.00038 0.00576 0.00
    \" 40, 0.890293, 0.5000, 0.78871, 0.00038, 0.00576, 0.00483, 0,
    \"/home/det/p2_det/images/mpy_spec_scan83*\",
    \"\",
    \"Returning eta to 0.790293\",
    \"\",
  ],
  "file_size_bytes": 4257804,
  "last_modified_timestamp": 1749652145.1257138,
  "message": \"Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}
```

The eta scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "gaussian",  
  "x_column": "eta",  
  "y_columns": "pd5",  
  "scan_number": "83",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



Good! The peak is well-centered at $\eta = 0.7909^\circ$. This is very close to the current position. Let me do a finer chi scan:

Execute Command: dscan chi -0.02 0.02 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

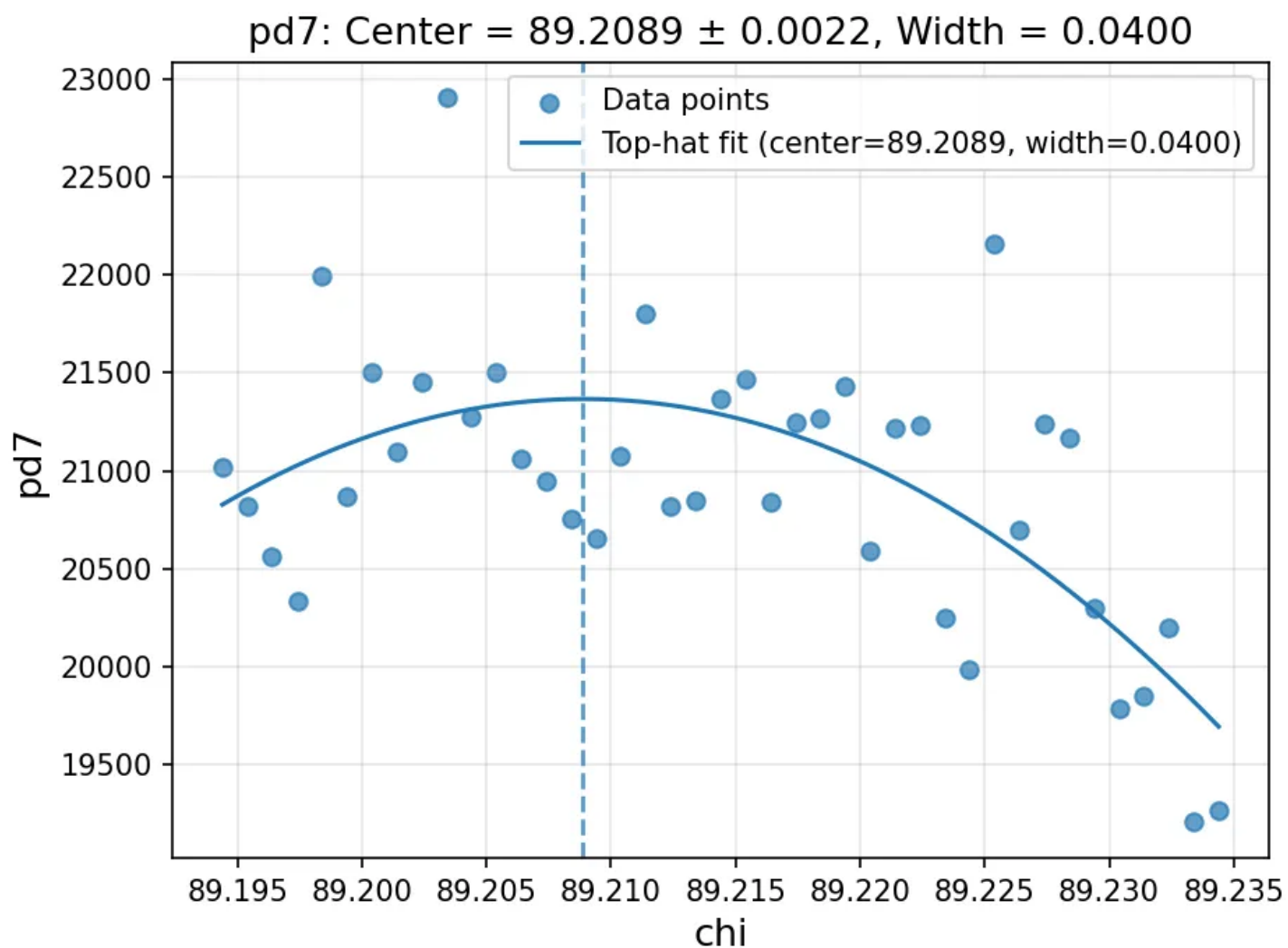
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 39, 89.2334, 0.5000, 0.80016, 0.0004, 0.00581, 0.0048, 0,  
    \"Shutter open.\",  
    \"Shutter closed.\",  
    " 40 89.2344 0.5 0.5 0.5 0.7981 0.0004 0.00576 0.0048  
    \"89.234395 1.0107876 -0.015088084 9.9873157 22793.069 0.79812 0.0004 0.00576 0.0048  
    \" 40, 89.2344, 0.5000, 0.79812, 0.0004, 0.00576, 0.0048, 0,  
    \"/home/det/p2_det/images/mpy_spec_scan84*\",  
    \"\",  
    \"Returning chi to 89.2144\",  
    \"\",  
  ],  
  "file_size_bytes": 4301233,  
  "last_modified_timestamp": 1749652222.1859477,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

The chi scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "tophat",  
  "x_column": "chi",  
  "y_columns": "pd7",  
  "scan_number": "84",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



The chi scan shows the peak is centered at 89.2089° . Let me move chi to this position:

Execute Command: umv chi 89.2089

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "1433.PSIC> umv chi 89.2089",  
    "",  
    "      chi ",  
    " 89.20115 ",  
    " 89.18937 ",  
    " 89.20891 ",  
    " 89.20891 ",  
    " 89.20891 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 4301336,  
  "last_modified_timestamp": 1749652279.2048607,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good. Now let me do a finer del scan:

Execute Command: dscan del -0.2 0.2 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

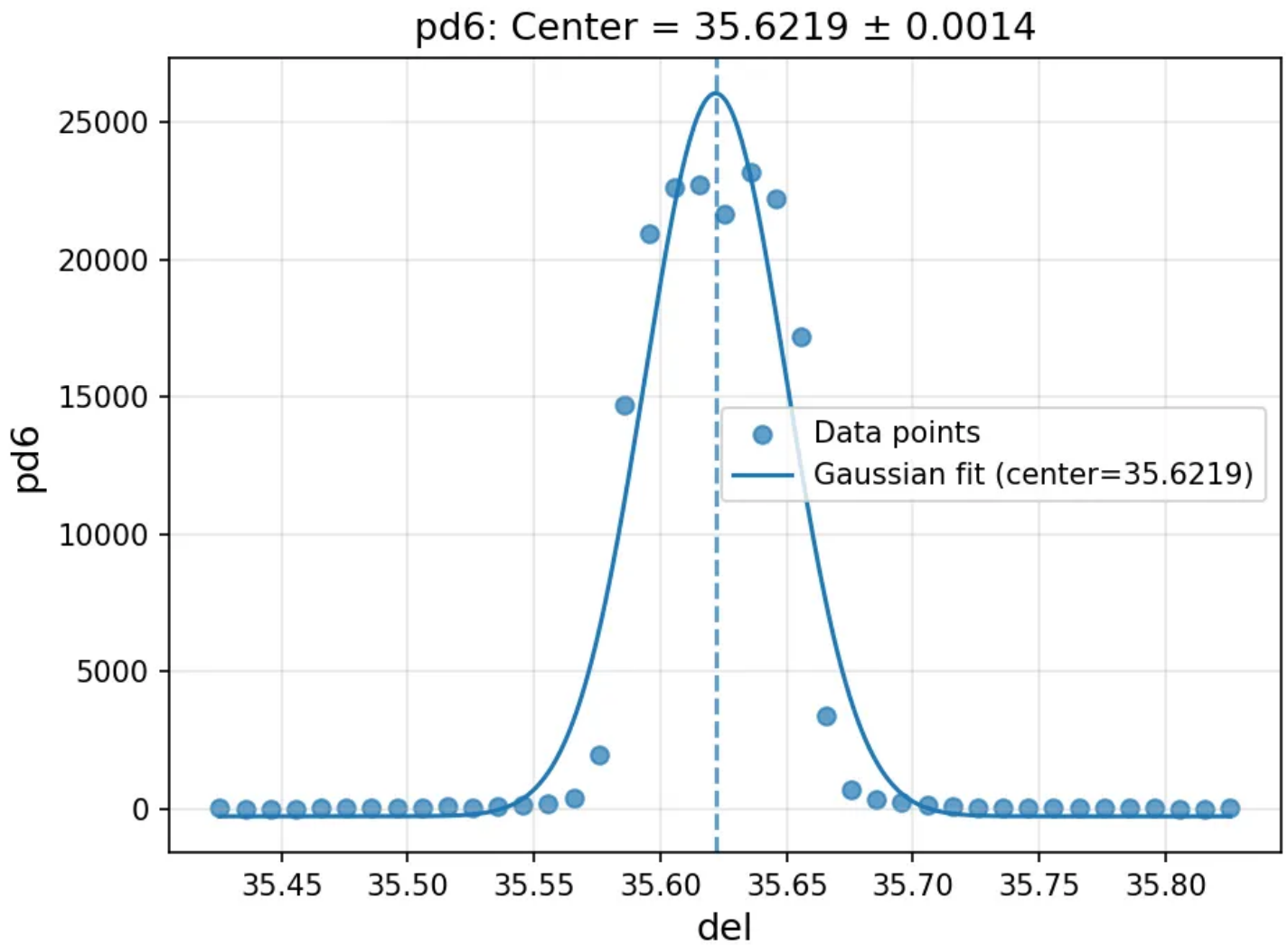
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 39, 35.8156, 0.5000, 0.796, 0.00043, 0.00579, 0.00486, 0,  
    "Shutter open.",  
    "Shutter closed.",  
    " 40 35.8256 0.5 0.5 0.5 0.7968 0.00039 0.00581 0.00486  
    "35.825605 1.0215776 -0.01339431 10.036553 22918.423 0.79682 0.00039 0.00581 0.0048  
    " 40, 35.8256, 0.5000, 0.79682, 0.00039, 0.00581, 0.00486, 0,  
    "/home/det/p2_det/images/mpy_spec_scan85*",  
    "",  
    "Returning del to 35.6256",  
    ""  
  ],  
  "file_size_bytes": 4344527,  
  "last_modified_timestamp": 1749652347.2649505,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

The del scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "gaussian",  
  "x_column": "del",  
  "y_columns": "pd6",  
  "scan_number": "85",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



Good! The peak is centered at $del = 35.6219^\circ$. This is very close to the current position. Let me do one final eta scan:

Execute Command: dscan eta -0.05 0.05 40 0.5

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

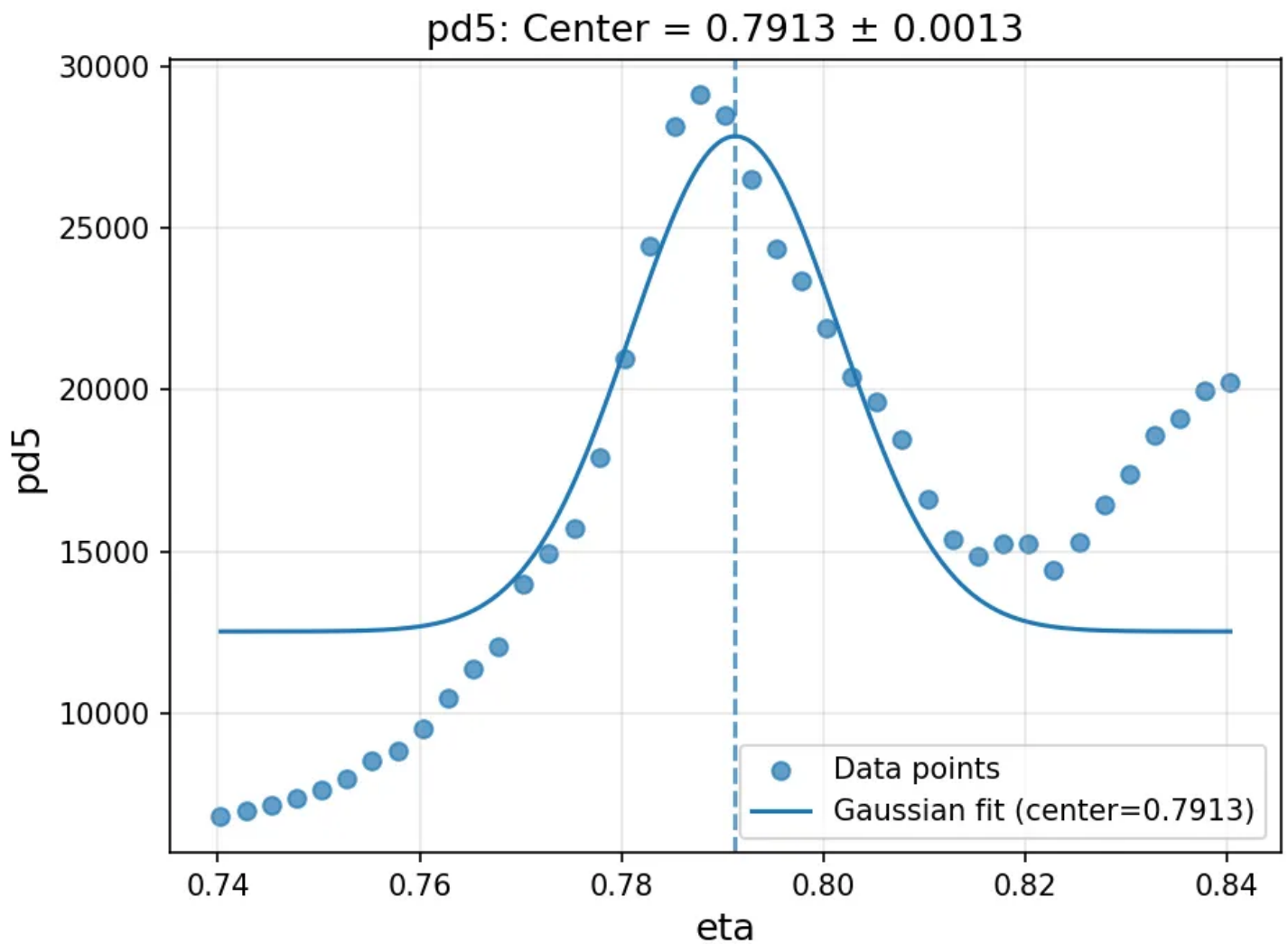
```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    " 39, 0.837793, 0.5000, 0.79199, 0.00036, 0.00578, 0.00483, 0,  
    "Shutter open.",  
    "Shutter closed.",  
    " 40 0.8403 0.5 0.5 0.5 0.7922 0.00038 0.00566 0.0048  
    "0.84029297 1.0068129 -0.013272303 9.9898027 23014.375 0.79224 0.00038 0.00566 0.00  
    " 40, 0.840293, 0.5000, 0.79224, 0.00038, 0.00566, 0.0048, 0,  
    "/home/det/p2_det/images/mpy_spec_scan86*",  
    "",  
    "Returning eta to 0.790293",  
    ""  
  ],  
  "file_size_bytes": 4387916,  
  "last_modified_timestamp": 1749652443.3284886,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

The final eta scan is complete. Let me visualize it:

read_and_plot_spec

Request

```
{  
  "fit_type": "gaussian",  
  "x_column": "eta",  
  "y_columns": "pd5",  
  "scan_number": "86",  
  "spec_file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\spec\\spec"  
}
```



Excellent! The peak is well-centered at $\eta = 0.7913^\circ$. This is very close to the current position. Let me move η to this final optimized position:

Execute Command: `umv eta 0.7913`

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log/logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "",  
    "1436.PSIC> umv eta .7913",  
    "",  
    "    eta ",  
    "  0.79131 ",  
    "  0.79131 ",  
    "  0.79131 ",  
    "  0.79131 ",  
    "",  
    ""  
  ],  
  "file_size_bytes": 4388005,  
  "last_modified_timestamp": 1749652512.3495936,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\  
}
```

Good! Now let me take a final detector image to verify the peak is well-centered:

Execute Command: pd exposure 1010_final_optimized 1.0

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 10  
}
```

Response

```
{  
  "status": "success",  
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",  
  "lines_requested": 10,  
  "lines_returned": 10,  
  "log_lines": [  
    "ROI_7_X1=277; ROI_7_Y1=7; ROI_7_X2=279; ROI_7_Y2=187;",  
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",  
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",  
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",  
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",  
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",  
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",  
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",  
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",  
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;"  
  ],  
  "file_size_bytes": 4389943,  
  "last_modified_timestamp": 1749652557.3633144,  
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
```

Let me check the current position:

Execute Command: wh

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{  
  "lines": 20  
}
```

Response

```

{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 20,
  "lines_returned": 20,
  "log_lines": [
    "ROI_8_X1=79; ROI_8_Y1=1; ROI_8_X2=479; ROI_8_Y2=193;",
    "ROI_9_X1=0; ROI_9_Y1=0; ROI_9_X2=0; ROI_9_Y2=0;",
    "ROI_10_X1=0; ROI_10_Y1=0; ROI_10_X2=0; ROI_10_Y2=0;",
    "ROI_11_X1=0; ROI_11_Y1=0; ROI_11_X2=0; ROI_11_Y2=0;",
    "ROI_12_X1=0; ROI_12_Y1=0; ROI_12_X2=0; ROI_12_Y2=0;",
    "ROI_13_X1=0; ROI_13_Y1=0; ROI_13_X2=0; ROI_13_Y2=0;",
    "ROI_14_X1=0; ROI_14_Y1=0; ROI_14_X2=0; ROI_14_Y2=0;",
    "ROI_15_X1=0; ROI_15_Y1=0; ROI_15_X2=0; ROI_15_Y2=0;",
    "ROI_16_X1=0; ROI_16_Y1=0; ROI_16_X2=0; ROI_16_Y2=0;",
    "",
    "1438.PSIC> wh",
    "",
    "H K L = 1.0098 -0.013289 9.9874\t Lambda = 0.7749 Two Theta = 35.626",
    "",
    "    Alpha      Beta      Psi      Tau      Qaz      Naz      Omega",
    " 29.6817 -24.3979 118.7735 82.2872 90.0000 -178.8035 -17.0215",
    "",
    "    del      eta      chi      phi      nu      mu ",
    " 35.62561    0.79131 89.20891 -2.87980 0.00000 0.00000 ",
    ""
  ],
  "file_size_bytes": 4390307,
  "last_modified_timestamp": 1749652590.373843,
  "message": "Successfully read 20 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\
}

```

Perfect! The peak is well-centered at H K L = 1.0098, -0.013289, 9.9874, which is essentially (1,0,10). The two-theta value is 35.626°.

Now I need to visualize the final detector image and then optimize the lattice parameter a based on this measured two-theta value:

explore_directory

Request

```
{
  "max_depth": 1,
  "file_pattern": "1010_final_optimized*.raw",
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"
}
```

Response

Directory scan for: X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images

Scan time: 2025-06-11 07:36:59

 images

===== RECENT FILES =====

Let me check all recent files:

explore_directory

Request

```
{
  "max_depth": 1,
  "show_recent": true,
  "file_pattern": "*.raw",
  "directory_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images"
}
```

Response

Directory scan for: X:\bl17-2\2025_06_Chen\project_roots\Co3Sn2S2\images
Scan time: 2025-06-11 07:37:05

 images

-  003_initial_061125-032459.raw (1.1 MB), modified 3 hours ago
-  006_eta_centered_061125-044426.raw (1.1 MB), modified 2 hours ago
-  006_eta_centered_061125-063210.raw (1.1 MB), modified 49 minutes ago
-  006_eta_optimized_061125-025321.raw (1.1 MB), modified 4 hours ago
-  006_final_061125-040903.raw (1.1 MB), modified 3 hours ago
-  006_final_optimized_061125-031948.raw (1.1 MB), modified 4 hours ago
-  006_final_optimized_061125-050052.raw (1.1 MB), modified 2 hours ago
-  006_final_optimized_061125-060916.raw (1.1 MB), modified 1 hour ago
-  006_final_optimized_061125-064812.raw (1.1 MB), modified 33 minutes ago
-  006_initial_061125-024503.raw (1.1 MB), modified 4 hours ago
-  006_initial_061125-034550.raw (1.1 MB), modified 3 hours ago
-  006_initial_061125-044109.raw (1.1 MB), modified 2 hours ago
-  0114_initial_061125-041319.raw (1.1 MB), modified 3 hours ago
-  011_initial_061125-033022.raw (1.1 MB), modified 3 hours ago
-  1010_final_optimized_061125-052442.raw (1.1 MB), modified 1 hour ago
-  1010_final_optimized_061125-071312.raw (1.1 MB), modified 8 minutes ago
-  1010_initial_061125-051129.raw (1.1 MB), modified 2 hours ago
-  1010_initial_search_061125-065247.raw (1.1 MB), modified 29 minutes ago
-  initial_006_search_061125-055400.raw (1.1 MB), modified 1 hour ago
-  initial_check_061125-005204.raw (1.1 MB), modified 6 hours ago
-  optimized_006_061125-010814.raw (1.1 MB), modified 6 hours ago
-  search_006_061125-005441.raw (1.1 MB), modified 6 hours ago
-  search_1014_061125-011920.raw (1.1 MB), modified 6 hours ago
-  test_006_initial_061125-062853.raw (1.1 MB), modified 53 minutes ago

===== RECENT FILES =====

Most recent *.raw files:

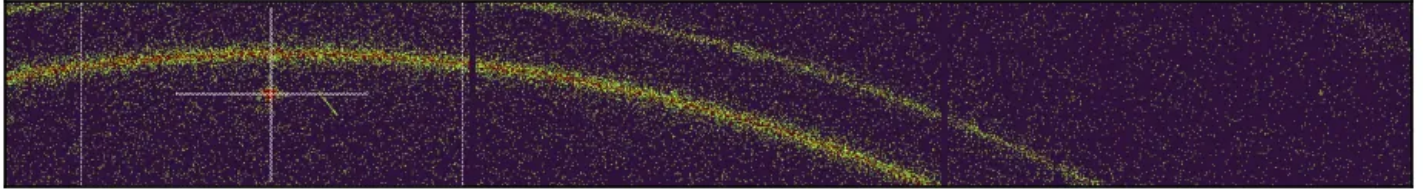
-  1010_final_optimized_061125-071312.raw (modified: 2025-06-11 07:28:08)
-  1010_initial_search_061125-065247.raw (modified: 2025-06-11 07:07:43)
-  006_final_optimized_061125-064812.raw (modified: 2025-06-11 07:03:09)
-  006_eta_centered_061125-063210.raw (modified: 2025-06-11 06:47:07)
-  test_006_initial_061125-062853.raw (modified: 2025-06-11 06:43:49)

I see the file 1010_final_optimized_061125-071312.raw. Let me visualize it:

read_and_plot_image

Request

```
{  
  "image_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\images\\1010_final_  
}
```



Excellent! I can see the (1,0,10) peak is well-centered in the detector. Now I'll optimize the lattice parameter a based on the measured two-theta value of 35.626° :

optimize_lattice_parameter

Request

```
{  
  "H": 1,  
  "K": 0,  
  "L": 10,  
  "a": 5.3574,  
  "b": 5.3574,  
  "c": 13.1646,  
  "beta": 90,  
  "alpha": 90,  
  "gamma": 120,  
  "store_as": "optimized_lattice_final",  
  "session_id": "6e65513f-2af4-477e-9e35-fe9ba5ab1bd1",  
  "wavelength": 0.7749,  
  "target_param": "a",  
  "two_theta_measured": 35.626  
}
```

Response

Lattice Parameter Optimization Results (Session: 6e65513f-2af4-477e-9e35-fe9ba5ab1bd1):

Original Parameters:

$a = 5.357400 \text{ \AA}$, $b = 5.357400 \text{ \AA}$, $c = 13.164600 \text{ \AA}$
 $\alpha = 90.000^\circ$, $\beta = 90.000^\circ$, $\gamma = 120.000^\circ$

Optimized Parameters:

$a = 5.361825 \text{ \AA}$, $b = 5.357400 \text{ \AA}$, $c = 13.164600 \text{ \AA}$
 $\alpha = 90.000^\circ$, $\beta = 90.000^\circ$, $\gamma = 120.000^\circ$

Optimization Details:

Target parameter: a
Original value: 5.357400
Optimized value: 5.361825
Change: 0.004425 (0.08%)

Peak: (1.0, 0.0, 10.0)
Measured 2θ : 35.626°
d-spacing observed: $1.266543 \text{ \AA}$
d-spacing calculated: $1.266544 \text{ \AA}$
d-spacing error: $0.00000003 \text{ \AA}$

Optimization successful: True

Result stored as 'optimized_lattice_final' in session 6e65513f-2af4-477e-9e35-fe9ba5ab1

Good! The optimized a lattice parameter is $5.3618 \text{ \AA}$. Since this is a hexagonal system, I should update both a and b to the same value:

Execute Command: setlat 5.3618 5.3618 13.1646 90 90 120

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 10
}
```

Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 10,
  "lines_returned": 10,
  "log_lines": [
    "",
    "      del      eta      chi      phi      nu      mu ",
    " 35.62561    0.79131   89.20891   -2.87980    0.00000    0.00000 ",
    "",
    "",
    "1439.PSIC> setlat 5.3618 5.3618 13.1646 90 90 120",
    "#C Wed Jun 11 07:16:22 2025.  g_aa reset from 5.3574 to 5.3618.",
    "#C Wed Jun 11 07:16:22 2025.  g_bb reset from 5.3574 to 5.3618.",
    "Can't find orientation matrix: Reflections are parallel.",
    ""
  ],
  "file_size_bytes": 4390545,
  "last_modified_timestamp": 1749652746.4183414,
  "message": "Successfully read 10 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
}
```

Good! The lattice parameters have been updated. Now let me set this as the secondary orientation reflection:

Execute Command: or1 1 0 10

Prompt:

Please read the log and continue.

Response:

read_log

Request

```
{
  "lines": 20
}
```

Response

```
{
  "status": "success",
  "file_path": "X:\\bl17-2\\2025_06_Chen\\project_roots\\Co3Sn2S2\\log\\logfile.log",
  "lines_requested": 20,
  "lines_returned": 20,
  "log_lines": [
    "",
    "      del      eta      chi      phi      nu      mu ",
    " 35.62561    0.79131  89.20891  -2.87980    0.00000    0.00000 ",
    "",
    "",
    "1439.PSIC> setlat 5.3618 5.3618 13.1646 90 90 120",
    "#C Wed Jun 11 07:16:22 2025.  g_aa reset from 5.3574 to 5.3618.",
    "#C Wed Jun 11 07:16:22 2025.  g_bb reset from 5.3574 to 5.3618.",
    "Can't find orientation matrix: Reflections are parallel.",
    "",
    "",
    "1440.PSIC> or1 1 0 10",
    "#C Wed Jun 11 07:17:23 2025.  g_h1 reset from 0 to 1.",
    "#C Wed Jun 11 07:17:23 2025.  g_l1 reset from 1 to 10.",
    "#C Wed Jun 11 07:17:23 2025.  g_u10 reset from 50 to 35.6256.",
    "#C Wed Jun 11 07:17:23 2025.  g_u11 reset from 0 to 0.791309.",
    "#C Wed Jun 11 07:17:23 2025.  g_u12 reset from 90 to 89.2089.",
    "#C Wed Jun 11 07:17:23 2025.  g_u13 reset from 0 to -2.8798.",
    "(UB recalculated from orientation reflections and lattice.)",
    ""
  ],
  "file_size_bytes": 4390985,
  "last_modified_timestamp": 1749652807.4373186,
  "message": "Successfully read 20 lines from X:\\bl17-2\\2025_06_Chen\\project_roots\\"
}
```

Excellent! The UB matrix has been calculated from the two orientation reflections. Now I need to verify the alignment by checking if I can find additional peaks at their predicted positions. Let me

check some verification peaks.

Let me use the ca command to calculate positions for another peak, such as (0,1,11):

Execute Command: `ca 0 1 11`

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