Powgen User Manual for Data Access

This document contains a detailed description of how to access Powgen data. To access data from a proposal, you must be listed as a team member on that proposal, and you must login with the XCAMS ORNL account with the same email as that listed on the proposal. This is the same as your account for IPTS. To create an account or reset your password, go to https://user.ornl.gov/Account/Login.aspx.

ONCat

The ORNL Neutron Catalog website (ONCat) is the primary way to access and download neutron data and metadata.

1. Go to <u>https://oncat.ornl.gov/</u> and login with your XCAMS credentials using the Login button in the upper right corner (Figure 1).



Figure 1. ONCat main screen, showing the Login button in the top-right and the Browse button at the bottom.

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2. Click Browse to bring up a list of instruments at HFIR and SNS and select POWGEN from the SNS list on the right (Figure 2).

🌻 ONCat	Instruments		(Kirkham, Melanie)	Logout
High Flux	FIR K Isotope Reactor	Spall	SINS Pation Neutron Source	Ce
CG-3 BIO-SANS		BL-1B NOMAD	le Differentemeter	> 1
Biological Small-Angle Neutron	Scattering Instrument	Nanoscale-Ordered Materia	is Diffactometer	
CG-4B CNPDB Cold Neutron Polarization Devel	opment Beamline	NOW-B NOWB		>
CG-4C CTAX Cold Neutron Triple-Axis Spectro	ometer	NOW-D NOWD		>
CG-1B DEV BEAM	Line	BL-15 NSE Neutron Spin Echo Spectro	meter	>
HB-3A FOUR-CIRCLE Four-Circle Diffractometer	:	BL-11A POWGEN Powder Diffractometer		>
		BL-17 SEQUOIA		

Figure 2. ONCat Instruments screen, showing the link to Powgen data.

3. On the Powgen page (Figure 3), click Experiments to bring up a list of proposals to which you have access. Then click the Proposal you wish to access.



Figure 3. ONCat POWGEN screen header, showing the Experiments button.

- 4. On the Proposal page, you may click Runs to see <u>metadata</u> for that proposal (Figure 4).
 - 4.1. The Download as CSV link in the top right initiates a download of the metadata.
 - 4.2. Clicking the plot icon in the leftmost column will take you to the monitor page (<u>https://monitor.sns.gov</u>) for that run.

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4.3. Clicking the Sample ID link will bring up a list of runs collected on that sample across different proposals and instruments.

🗘 ONCat		Instruments > SNS / PG3 > E	xperiments > IP	TS-32378 > Runs				(Kirkham, Melanie)
PC	POWGEN Info Download as CSV						Download as CSV	
_		Run				Sample		
ţ.	D	Title	Start Time	End Time	Duration	Proton Charge (C)	ID	Name
5	# 58,342 >	Empty quartz tube in PAC 10mm	2024-11-21 11:38:31	2024-11-21 14:29:07	02:50:36	12.53	100,055 >	Quartz tube in 10 mm PAC can
5	# 58,341 >	2024B Remeasure V rod-New Furnace CWL=0.8A on	2024-11-21 08:29:55	2024-11-21 11:15:04	02:45:09	12.80	11,534 >	Vanadium Rod
5	# 58,340 >	2024B quick test empty MICAS-New Furnace CWL=0	2024-11-21 08:01:53	2024-11-21 08:20:35	00:18:42	1.47		-
5	# 58,331 >	2024B long calibration 8mm PAC empty HR on Nov 1	2024-11-19 16:40:07	2024-11-19 20:54:18	04:14:10	20.00	95,066 >	Empty 8 mm can for new MICAS stick
5	# 58,330 >	2024B long calibration 8mm PAC empty HR on Nov 1	2024-11-19 16:32:42	2024-11-19 16:35:14	00:02:31	0.20	95,066 >	Empty 8 mm can for new MICAS stick
5	# 58,329 >	quick diamond	2024-11-19 16:00:48	2024-11-19 16:16:23	00:15:34	1.23	87,972 >	Diamond
<u></u>	# 58,328 >	quick diamond	2024-11-19 15:48:23	2024-11-19 15:54:43	00:06:20	0.50	87,972 >	Diamond

Figure 4. ONCat Proposal metadata screen showing a list of runs. Red arrows point out (left-to-right) SNS monitor link, link to list of all runs for a sample, and how to download all the metadata as a CSV file.

- 5. On the Proposal page, you may click Download to <u>download neutron data</u> (Figure 5).
 - 5.1. On the Data Download page, click the green magnifying glass button under Brower (HTTPS).
 - 5.2. On the following page (Figure 6), use the folder structure to navigate to /SNS/PG3/IPTS-XXXXX/shared/autoreduce.
 - 5.3. Check the boxes next to files you wish to download. File types are covered below.
 - 5.4. Press the green Download button in the bottom right, then the Download button on the popup window to initiate download of a zipped archive of the selected files.
 - 5.5. Alternatively, the Data Download page has instructions for connecting to the analysis cluster to transfer your data directly via SFTP (FileZilla, Cyberduck), SSH or Globus Connect.



Figure 5. ONCat Proposal and Data Download page, showing how to get to the Browser Download screen.

Filter by Path		Expand All / C	ollapse All	=×	=%
2.2					
En SNS/					
🖻 PG3/					
D IPTS-32378/ 8/2k		Updated 1 hour ago. 2024-12-	-18 06:03 3	18.3 GB	
🛅 images/ (0/0)		2024-06-	07 06:00	0 Bytes	
🛅 nexus/ (0/187)		2024-11-	21 09:29 2	86.2 GB	
🖻 shared/ (8/1k)		2024-12-	-18 06:03	32.1 GB	
🛅 GenII-test/ (0/3)		2024-12-	18 06:03	1.7 MB	
autoreduce/ (8/1k)		2024-12-	06 07:18	32.1 GB	
.~lock.PG3_IPTS-32378_runsummary.	SV#	2024-07-	16 12:55	90 B	
TSRed/ (0/0)		2024-09-	06 12:56	0 Bytes	
PG3_56569-1.dat		2024-07-	22 12:39	253 KB	~
PG3_56569-1.xye		2024-07-	22 12:39	253 KB	~
PG3_56569.gr		2024-07-	22 12:39 3	26.7 KB	~
PG3_56569.gsa		2024-07-	22 12:39 3	84.5 KB	~
PG3_56569.py		2024-07-	22 12:39	749 B	~
PG3_56569_SQ.nxs		2024-07-	22 12:39	113 MB	~
PG3_56570-2.dat		2024-07-	22 12:39 2	04.9 KB	
PG3_56570-2.xye		2024-07-	22 12:39 2	04.9 KB	
PG3_56570.gsa	The data with the state	2024-07-	22 12:39 3	11.4 KB	
PG3_56570.py	Update File List	2024-07-	22 12:39	749 B	~
elected file(s).				Unche	ck A

Figure 6. ONCat Browser Download screen. Navigate to /SNS/PG3/IPTS-XXXXX/shared/autoreduce, check the boxes on the right for the files to be downloaded, then press the Download button.

Data Formats and Parameter Files

Data are automatically reduced to GSAS, FullProf and Topas formats using the default parameters. Those data are found in the /shared/autoreduce/ folder.

- <u>Extension .gsa for GSAS-II</u>: File header contains the wavelength. Please use the corresponding GSAS instprm parameter file for refinements.
- <u>Extension .dat for FullProf or Jana</u>: The filename has the bank number appended after the run number. For example, PG3_24759-2.xye is run number 24759 collected with bank 2. Please use the same bank parameter file for refinements.
- <u>Extension . xye for Topas</u>: As with the FullProf data, the filename has the bank number appended after the run number.
- Extensions .gr and <u>SQ.nxs</u>: These files are for PDF analysis.
- Extension .py: These files contain the parameters used for autoreduction.
- <u>File PG3_IPTS-XXXXX_runsummary.csv</u>: This comma-separated-variable file contains meta-data about each run, such as sample temperature and wavelength, and may be opened in any spreadsheet program.

Parameter files for various Rietveld refinement programs (GSAS-II, FullProf, JANA and Topas) can be downloaded from the table titled "Data Reduction and Analysis by Run Cycle" on the User Guidance page of the Powgen website (<u>https://neutrons.ornl.gov/powgen/users</u>). Be sure to pick the correct time range.