Data Description (Starting 2017) for POWGEN

POWGEN will provide multiple options for data after the upgrade.

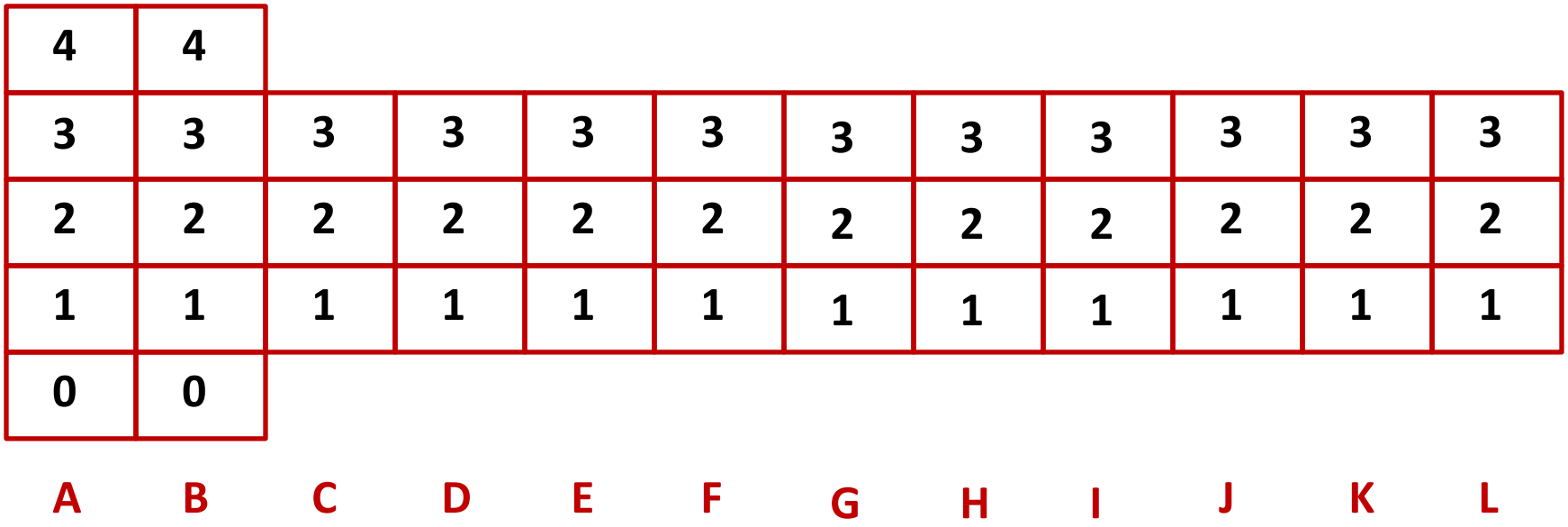

Figure 1: Detector layout for South side of instrument.

Calibrated Wavelengths for cycle 2017-A/B

Frequency (Hz)	WL center	WL min	WL max	d_{min}	d_{max}	Q_{min}	Q_{max}
60	0.700	0.167	1.233	0.0838	8.2000	0.7662	74.9564
60	1.500	0.967	2.033	0.4854	14.0000	0.4488	12.9449
60	2.665	2.132	3.198	1.0701	22.2000	0.2830	5.8714

Table of 2Θ and available d-space in each column of detectors for the calibrated wavelengths

Center Wavelength			0.7		1.5		2.665	
	2Θ max	2Θ min	d min	d max	d min	d max	d min	d max
A (1-5)	169.0824	142.9060	0.1005	0.6329	0.5023	1.0548	1.0874	1.6692
B (6-10)	149.5326	128.4971	0.1036	0.6662	0.5182	1.1103	1.1219	1.7570
C (11-13)	131.2671	114.5567	0.1098	0.7132	0.5489	1.1886	1.1884	1.8810
D (14-16)	114.5379	99.3627	0.1189	0.7869	0.5944	1.3115	1.2868	2.0755
E (17-19)	99.0051	85.1335	0.1315	0.8870	0.6575	1.4783	1.4235	2.3394
F (20-22)	84.7212	71.6829	0.1484	1.0247	0.7421	1.7078	1.6066	2.7026
G (23-25)	71.5049	59.0582	0.1711	1.2174	0.8557	2.0290	1.8527	3.2108
H (26-28)	59.0424	47.2581	0.2029	1.4970	1.0147	2.4949	2.1969	3.9482
I (29-31)	47.4001	36.0728	0.2488	1.9379	1.2439	3.2298	2.6931	5.1111
J (32-34)	36.3900	25.4916	0.3203	2.7195	1.6013	4.5326	3.4667	7.1728
K (35-37)	26.1025	15.4801	0.4428	4.4551	2.2141	7.4251	4.7936	11.7502
L (38-40)	16.5996	6.1222	0.6927	11.2358	3.4637	18.7264	7.4990	29.6345

Starting this cycle we will start supporting GSAS-II. All refinements done by instrument staff will be available for users and will be stored in

/SNS/PG3/shared/CALIBRATION/2017_1_2_11A_CAL/GSAS

/SNS/PG3/shared/CALIBRATION/2017_1_2_11A_CAL/FP

/SNS/PG3/shared/CALIBRATION/2017_1_2_11A_CAL/GSAS-II

Following options will be used for autoreduced data which will be stored in the following folder.

/SNS/IPTS-#/shared/autoreduce

Option 1: 2 Histogram/ dataset:

Histogram 1: detectors A-H + I2 + J2 + K2 + L2 (32 detectors)

Histogram 2: detectors I1 + I3 + J1 + J3 + K1 + K3 + L1 + L3 (8 detectors)

This is our standard option which takes into account that some of our out of plane detectors especially in the forward scattering locations have lower resolution than the rest of the detectors. Each data set (for a specified lambda) will have two histograms.

- GSAS data PG3_run#.gsa Banks 1 and 2 for 0.7 Å, 3 and 4 for 1.5 Å, 5 and 6 for 2.665Å
  - Parameter file PG2017AB_HR60_2B.prm
- GSAS-II: standard gsas files can be used for GSAS-II
  - Parameter files are 2017AB_HR60b**n**_2B.instprm where n=1-6, 2 datasets for each wavelength
- Fullprof data PG3_run#-**n**.dat and IRF file PG2017AB_HR60b**n**_2B where n=1-6, 2 datasets for each wavelength.
- Topas same as Fullprof with extension .xye instead of .dat

Option 2: 1 histogram/dataset:

Histogram: detectors A-L all 40 detectors.

This option is sufficient for samples which have broader peaks, where the degraded resolution is an acceptable trade-off for the convenience of working with a single data set with better overall counting statistics.

- GSAS data ALL_PG3_run#.gsa Banks 1, 2 and 3 for the three separate wavelengths.
    - Parameter file PG2017AB_HR60_ALL.prm
- GSAS-II: standard gsas files can be used for GSAS-II
    - Parameter files are 2017AB_HR60b**n**_ALL .instprm where n=1-3, 1 datasets for each wavelength
- Fullprof data ALL_PG3_run#-**n**.dat and IRF file PG2017AB_HR60b**n**_ALL where n=1, 2 and 3 for the three separate wavelengths.
- Topas same as Fullprof with extension .xye instead of .dat
- Raw data for PDF analysis PG3_run#.getn (this data set is the raw time focused data set with no normalization).

Option 3: Additional Data:

Histogram: detectors A-L in plane (A2, B2, C2……..K2, L2) only (12 detectors)

This dataset is provided to look at the higher resolution data for looking at splitting that are subtle and not visible from the other two options.

- GSAS data IP_PG3_run#.gsa Banks 1, 2 and 3 for the three separate wavelengths.
    - Parameter file PG2017AB_HR60_IP.prm
- GSAS-II: standard gsas files can be used for GSAS-II
    - Parameter files are 2017AB_HR60b**n**_IP.instprm where n=1-3, 1 datasets for each wavelength
- Fullprof data IP_PG3_run#-**n**.dat and IRF file 2017AB_HR60b**n**_IP where n=1, 2 and 3 for the three separate wavelengths.
- Topas same as Fullprof with extension .xye instead of .dat

For any other option for grouping detectors please discuss with instrument team members.