



Nb.	Data Type	Format	Description / Origin	Volume
1a	Description of sample preparation	Handwritten notes	Description, experiment conditions and observations during sample preparation. Created while experiment is carried out.	-
1b	Description of sample preparation	.pdf	1a are scanned once a week.	10-50 MB
1c	Description of sample preparation	.txt	1b are converted into text using the handwriting recognition feature of Microsoft OneNote. Additional metadata are added to the file as described in section 1.3 for files 1c .	100-150 KB
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2a	X-ray diffraction data	.xrdml	Raw file created by PANanalytical X-ray diffractometer (includes the instrument type and measurement settings).	1-2 MB
2b	X-ray diffraction data	.asc	2a are background corrected and converted to .asc files using Malvern Panalytical Highscore Plus (version 4.6a).	3-5 MB
2c	X-ray diffraction data	.opj	2b are imported in Origin2018b and different plots are created for further analysis.	50-150 MB
2d	X-ray diffraction data	.svg	Plots created from 2c are exported from Origin2018b as vector files.	100-200 MB
2e	X-ray diffraction data	.cif	2a raw files are converted to crystallographic information files (CIF) using Malvern Panalytical Highscore Plus (version 4.6a).	10-50 MB