

# The LaueUtil toolkit for Laue Photocrystallography:

## I. Rapid orientation matrix determination for intermediate size unit-cell Laue data

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Table S1. Angular discrepancies derived from Me matrix for all tested data sets.

Data set	Logfile	Type	Laser $\mu$ J/ mm <sup>2</sup>	phi spacing °	Precognition Mean Discrepancy °	Precognition Max Discrepancy °	LaueUtil Mean Discrepancy °	LaueUtil Max Discrepancy °
CuBF4T_02	dark	dark	0	1	0.14	0.29	0.28	0.35
	laser1	OFF/ON/OFF x 10 x phi	0.3	1	0.12	0.26	0.26	0.34
	laser2	ON/OFF x 10 x phi	0.4	1	0.12	0.22	0.15	0.26
	laserpower1	ON/OFF x 10 x phi	0.5	1	0.57	0.93	0.30	0.78
	samephi	samephi	0	0	0.01	0.04	0.25	0.28
	samephi1	samephi	0	0	0.03	0.06	0.27	0.30
CuBF4T_03	laserpower1	ON/OFF x 10 x phi	0.1	1	0.10	0.33	0.59	0.64
	laserpower2	ON/OFF x 10 x phi	0.6	1	0.07	0.25	0.21	0.26
	laserpower3	ON/OFF x 10 x phi	0.7	1	0.16	0.27	0.15	0.28
	laserpower4	ON/OFF x 10 x phi	0.9	1	0.15	0.29	0.27	0.32
CuBF4T_04	laserpower1	ON/OFF x 10 x phi	0.7	1	0.02	0.05	0.11	0.34
	laserpower2	ON/OFF x 10 x phi	0.8	1	0.05	0.27	0.18	0.35
	laserpower3	ON/OFF x 10 x phi	0.9	1	0.13	0.22	0.14	0.22
	laserpower4	ON/OFF x 10 x phi	1.1	1	7.95	21.12	crystal slipped on mount	
	laserpower5	ON/OFF x 10 x phi	1.3	1	9.15	22.06		
CuBF4T_06	laserpower1	ON/OFF x 10 x phi	1.5	1	0.08	0.12	0.24	0.30
CuBF4T_07	dark	dark	0	1	0.12	0.22	0.15	0.25
	laser1	ON/OFF x 10 x phi	0.9	1	0.16	0.27	0.11	0.20
	laser2	ON/OFF x 10 x phi	1.1	2	0.12	0.23	0.15	0.20
CuBF4T_09	dark	dark	0	2	0.16	0.36	0.21	0.25
	laser1	ON/OFF x 10 x phi	0.7	2	0.19	0.33	0.33	0.54
	laser2	ON/OFF x 10 x phi	0.8	2	0.17	0.36	0.36	0.58
CuBF4T_10	dark	dark	0	2	0.06	0.11	0.12	0.18
	laser1	ON/OFF x 10 x phi	0.6	2	1.94	4.30	1.93	4.27
	laser2	ON/OFF x 10 x phi	0.7	2	1.32	7.42	1.31	7.35
CuBF4M_01	dark1	dark	0	1	0.09	0.17	0.11	0.12
	samephi	samephi	0	0	0.01	0.01	0.10	0.11

CuBF4M_02	dark	dark	0	2	0.10	0.22	0.15	0.22
	laserpower1	ON/OFF x 10 x phi	0.4	1	0.09	0.16	0.09	0.16
	laserpower2	ON/OFF x 10 x phi	0.6	1	0.05	0.09	0.06	0.13
	laserpower3	ON/OFF x 10 x phi	0.8	1	0.07	0.11	0.11	0.14
	laserpower4	ON/OFF x 10 x phi	1	1	0.19	0.23	0.10	0.13
	laserpower5	ON/OFF x 10 x phi	1.2	1	0.21	0.34	0.10	0.19
CuBF4M_03	dark	dark	0	2	0.09	0.17	0.27	0.36
	laser2	ON/OFF x 10 x phi	0.6	2	0.96	1.21	0.22	1.06
CuBF4M_04	dark	dark	0	2	0.09	0.20	0.11	0.18
	laser1	ON/OFF x 10 x phi	0.7	2	8.66	10.07	1.42	9.98
CuBF4M_05	dark	dark	0	2	0.08	0.18	0.12	0.17
	laser3	ON/OFF x 10 x phi	0.5	2	0.16	0.22	0.08	0.21
	laser4	ON/OFF x 10 x phi	0.7	2	0.12	0.27	0.07	0.23
CuTRI_01	dark	dark	0	1	0.14	0.31	0.26	0.45
	samephi	samephi	0	0	0.01	0.05	0.15	0.24
CuTRI_02	dark	dark	0	1	0.18	0.40	0.19	0.39
	laserpower1	ON/OFF x 10 x phi	0.7	1	0.09	0.16	0.15	0.22
	laserpower3	ON/OFF x 10 x phi	1.1	1	0.07	0.14	0.14	0.22
	laserpower4	ON/OFF x 10 x phi	1.3	1	0.07	0.14	0.15	0.22
	laserpower5	ON/OFF x 10 x phi	1.5	1	0.06	0.13	0.17	0.23
CuTRI_03	dark	dark	0	1	0.15	0.33	0.17	0.22
	laser1	ON/OFF x 10 x phi	1.1	1	9.95	30.23	crystal slipped on mount	
CuTRI_04	dark	dark	0	1	0.10	0.20	0.12	0.20
	laser1	ON/OFF x 10 x phi	0.9	1	0.95	1.14	0.16	1.04
CuTRI_05	dark	dark	0	1	0.08	0.15	0.06	0.10
	laser1	ON/OFF x 10 x phi	0.8	2	2.21	2.65	0.50	2.25
CuIpip06	dark	dark	0	1	0.10	0.17	0.07	0.15
	laser1	ON/OFF x 10 x phi	0.6	1	0.09	0.12	0.04	0.07
	laser2	ON/OFF x 10 x phi	0.8	1	0.12	0.19	0.14	0.28
RhPNP_27	dark	dark	0	1	0.19	0.34	0.14	0.23
	laser1	ON/OFF x 10 x phi	0.6	5	0.19	0.33	0.25	0.41