

ZTm123

** PROGRAM FullProf.2k (Version 5.40 - Mar2014-ILL JRC) **

M U L T I -- P A T T E R N
Rietveld, Profile Matching & Integrated Intensity
Refinement of X-ray and/or Neutron Data

Date: 24/12/2017 Time: 11:40:50.690

=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 8.94
=> RF-factor : 9.60

Pattern# 1 Phase No: 1 Phase name: ZTm123

No. d-hkl	Code	H	K	L	Mult	Hw	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2
		CORR										
1	1	0	0	3	2	0.140698	0.520994	22.767	84.3	97.8	15.466	6375.3643
3.902686		1.000000										
2	1	0	1	0	2	0.140546	0.520345	22.931	65.1	63.9	1.550	4997.0293
3.875114		1.000000										
3	1	1	0	0	2	0.140234	0.519003	23.270	49.5	50.3	1.255	3913.0815
3.819361		1.000000										
4	1	0	1	1	4	0.139424	0.515437	24.172	5.5	3.8	1.258	234.2936
3.678846		1.000000										
5	1	1	0	1	4	0.139141	0.514160	24.495	13.6	8.2	3.371	599.9399
3.631042		1.000000										
6	1	0	1	3	4	0.133430	0.482380	32.535	355.0	345.0	9.921	28479.9023
2.749815		1.000000										
7	1	1	0	3	4	0.133298	0.481405	32.782	396.4	372.1	22.615	32315.7461
2.729679		1.000000										
8	1	1	1	0	4	0.133237	0.480940	32.899	410.7	417.1	6.752	33743.9922
2.720193		1.000000										
9	1	1	1	1	8	0.132785	0.477373	33.801	0.2	0.3	0.185	9.0317

												ZTm123
2.649621		1.000000										
10	1	1 1	2	8	0.131707	0.467142	36.390	4.4	5.0	1.587	223.0349	
2.466877		1.000000										
11	1	0 0	5	2	0.131101	0.459153	38.410	40.9	46.6	6.480	9401.0098	
2.341612		1.000000										
12	1	0 1	4	4	0.131076	0.458748	38.513	50.7	50.7	0.876	5863.7251	
2.335615		1.000000										
13	1	1 0	4	4	0.131026	0.457905	38.726	46.0	43.2	2.714	5376.3423	
2.323239		1.000000										
14	1	1 1	3	8	0.130720	0.451351	40.384	128.7	132.7	4.578	8253.7812	
2.231604		1.000000										
15	1	0 1	5	4	0.130721	0.432289	45.206	0.8	0.0	0.355	123.8848	
2.004131		1.000000										
16	1	1 0	5	4	0.130749	0.431549	45.394	1.1	0.4	0.329	181.0903	
1.996295		1.000000										
17	1	1 1	4	8	0.130763	0.431195	45.483	16.1	16.1	1.372	1343.4131	
1.992576		1.000000										
18	1	0 0	6	2	0.130959	0.427176	46.500	46.5	76.3	48.492	16288.0469	
1.951343		1.000000										
19	1	0 2	0	2	0.131042	0.425790	46.850	121.0	122.2	1.953	43130.7734	
1.937557		1.000000										
20	1	0 2	1	4	0.131223	0.423117	47.527	3.5	3.2	0.299	639.7550	
1.911558		1.000000										
21	1	2 0	0	2	0.131238	0.422921	47.576	115.0	105.8	8.553	42415.1055	
1.909681		1.000000										
22	1	2 0	1	4	0.131448	0.420279	48.245	3.3	1.1	0.892	625.5092	
1.884774		1.000000										
23	1	0 2	2	4	0.131928	0.415266	49.513	0.4	0.9	1.122	87.2643	
1.839423		1.000000										
24	1	2 0	2	4	0.132236	0.412512	50.210	0.4	0.6	0.678	85.8806	
1.815521		1.000000										
25	1	1 1	5	8	0.132866	0.407611	51.449	17.3	15.8	1.913	1902.6204	
1.774651		1.000000										
26	1	0 1	6	4	0.133457	0.403620	52.459	13.1	14.8	2.080	3004.3887	
1.742847		1.000000										
27	1	1 0	6	4	0.133561	0.402957	52.627	9.3	9.5	0.396	2139.3320	
1.737686		1.000000										
28	1	0 2	3	4	0.133608	0.402668	52.700	16.4	15.9	0.725	3794.8638	
1.735449		1.000000										
29	1	1 2	0	4	0.133767	0.401691	52.947	12.0	11.7	0.648	2807.2485	
1.727929		1.000000										
30	1	2 0	3	4	0.134047	0.400033	53.366	15.8	15.7	0.662	3753.8223	
1.715332		1.000000										

31	1	2	1	0	4	0.134102	0.399719	ZTm123 53.446	13.6	13.9	0.534	3251.9243
1.712971		1.000000										
32	1	1	2	1	8	0.134185	0.399245	53.566	2.2	2.4	0.288	258.6627
1.709413		1.000000										
33	1	2	1	1	8	0.134538	0.397288	54.061	1.0	0.2	0.484	121.8495
1.694926		1.000000										
34	1	0	0	7	2	0.135132	0.394195	54.843	10.5	17.5	11.795	5297.8574
1.672580		1.000000										
35	1	1	2	2	8	0.135577	0.392017	55.394	4.6	2.0	1.330	594.2109
1.657243		1.000000										
36	1	2	1	2	8	0.135985	0.390104	55.878	3.7	2.3	1.139	490.7143
1.644033		1.000000										
37	1	0	2	4	4	0.136948	0.385873	56.948	0.4	0.0	0.306	119.0539
1.615648		1.000000										
38	1	2	0	4	4	0.137557	0.383370	57.581	0.4	0.0	0.135	119.8176
1.599379		1.000000										
39	1	1	1	6	8	0.138109	0.381199	58.131	120.0	127.9	8.544	17276.9609
1.585568		1.000000										
40	1	1	2	3	8	0.138342	0.380310	58.356	138.8	145.8	7.439	20154.7207
1.579992		1.000000										
41	1	2	1	3	8	0.138838	0.378460	58.824	122.9	124.7	2.429	18163.6172
1.568531		1.000000										
42	1	0	1	7	4	0.140405	0.372972	60.212	12.3	11.3	1.217	3820.5974
1.535643		1.000000										
43	1	1	0	7	4	0.140587	0.372366	60.365	11.3	11.1	0.597	3526.0420
1.532109		1.000000										
44	1	0	2	5	4	0.142807	0.365395	62.129	16.3	15.5	1.256	5435.4077
1.492786		1.000000										
45	1	1	2	4	8	0.143105	0.364515	62.351	18.4	16.4	1.894	3085.6790
1.487992		1.000000										
46	1	2	0	5	4	0.143618	0.363019	62.730	15.8	16.2	0.726	5369.3755
1.479925		1.000000										
47	1	2	1	4	8	0.143717	0.362736	62.801	19.2	20.6	1.643	3264.2996
1.478407		1.000000										
48	1	0	0	8	2	0.144720	0.359915	63.515	0.7	0.1	0.478	504.1013
1.463507		1.000000										
49	1	1	1	7	8	0.147644	0.352256	65.453	30.2	34.4	5.017	5617.0542
1.424790		1.000000										
50	1	1	2	5	8	0.150681	0.345010	67.286	0.6	0.0	0.504	116.9276
1.390362		1.000000										
51	1	2	1	5	8	0.151437	0.343301	67.718	0.5	0.0	0.321	103.2731
1.382533		1.000000										
52	1	0	2	6	4	0.152197	0.341613	68.145	26.6	30.2	4.269	10734.2061

ZTm123												
1.374908		1.000000										
53	1	0 1	8	4	0.152792	0.340316	68.473	10.7	13.8	4.148	4341.3887	
1.369120		1.000000										
54	1	1 0	8	4	0.153054	0.339751	68.616	13.6	14.0	0.612	5567.9956	
1.366614		1.000000										
55	1	2 0	6	4	0.153241	0.339349	68.718	25.9	25.0	1.082	10618.6982	
1.364840		1.000000										
56	1	2 2	0	4	0.153748	0.338268	68.991	63.8	67.8	4.351	26420.5820	
1.360097		1.000000										
57	1	2 2	1	8	0.154750	0.336172	69.521	1.5	2.0	0.777	307.2238	
1.351011		1.000000										
58	1	2 2	2	8	0.157871	0.329924	71.102	0.3	0.5	0.695	56.5370	
1.324810		1.000000										
59	1	0 0	9	2	0.161051	0.323945	72.615	3.2	3.1	0.930	2903.1477	
1.300895		1.000000										
60	1	1 2	6	8	0.162085	0.322075	73.087	7.2	8.3	1.518	1663.2506	
1.293640		1.000000										

No. d-hkl	Code	H CORR	K	L	Mult	Hw	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2
61	1	0 3	0	2	0.162366	0.321572	73.215	2.7	2.9	0.336	2548.7627	
1.291705		1.000000										
62	1	1 1	8	8	0.162791	0.320817	73.406	0.5	0.6	0.130	114.6757	
1.288815		1.000000										
63	1	2 1	6	8	0.163012	0.320427	73.504	9.3	9.8	0.889	2160.7656	
1.287327		1.000000										
64	1	2 2	3	8	0.163460	0.319639	73.704	11.8	11.5	0.721	2779.7754	
1.284337		1.000000										
65	1	0 3	1	4	0.163524	0.319527	73.732	0.1	0.1	0.014	67.7532	
1.283914		1.000000										
66	1	3 0	0	2	0.165196	0.316640	74.462	2.3	1.6	0.874	2233.4045	
1.273120		1.000000										
67	1	0 2	7	4	0.166329	0.314727	74.946	7.6	10.7	4.320	3686.7461	
1.266094		1.000000										
68	1	3 0	1	4	0.166401	0.314607	74.977	0.3	0.4	0.172	130.7247	
1.265660		1.000000										
69	1	0 3	2	4	0.167113	0.313423	75.276	0.9	1.4	0.859	441.3830	
1.261363		1.000000										
70	1	2 0	7	4	0.167644	0.312549	75.497	7.5	10.7	4.782	3650.2266	
1.258219		1.000000										
71	1	3 0	2	4	0.170133	0.308538	76.512	1.0	0.0	0.677	504.3622	
1.244041		1.000000										

72	1	2	2	4	8	0.172104	0.305460	ZTm123 77.291	0.5	0.7	0.332	123.2604
1.233439	1	1.000000										
73	1	0	1	9	4	0.172138	0.305407	77.304	6.2	9.1	4.296	3168.1194
1.233257	1	1.000000										
74	1	1	0	9	4	0.172489	0.304867	77.441	6.2	8.6	3.250	3187.0708
1.231425	1	1.000000										
75	1	0	3	3	4	0.173490	0.303342	77.826	25.0	24.9	0.928	12909.2100
1.226282	1	1.000000										
76	1	1	3	0	4	0.174018	0.302546	78.028	29.3	29.6	0.886	15152.4561
1.223621	1	1.000000										
77	1	1	3	1	8	0.175362	0.300544	78.534	0.0	0.0	0.011	5.6775
1.216992	1	1.000000										
78	1	3	0	3	4	0.176752	0.298507	79.050	25.9	26.9	1.300	13711.3945
1.210347	1	1.000000										
79	1	3	1	0	4	0.176928	0.298250	79.115	28.1	28.3	0.753	14866.5557
1.209517	1	1.000000										
80	1	3	1	1	8	0.178316	0.296255	79.619	0.0	0.0	0.004	5.5985
1.203114	1	1.000000										
81	1	1	2	7	8	0.178609	0.295837	79.725	9.3	9.3	0.838	2494.8513
1.201784	1	1.000000										
82	1	1	3	2	8	0.179515	0.294557	80.049	0.4	0.4	0.041	119.1719
1.197736	1	1.000000										
83	1	2	1	7	8	0.179745	0.294233	80.131	9.8	8.5	1.355	2649.0081
1.196717	1	1.000000										
84	1	3	1	2	8	0.182603	0.290289	81.129	0.4	0.4	0.362	119.0406
1.184499	1	1.000000										
85	1	0	3	4	4	0.183270	0.289385	81.357	3.8	3.5	0.832	2112.7280
1.181748	1	1.000000										
86	1	2	2	5	8	0.184669	0.287512	81.831	13.6	12.1	1.614	3789.7727
1.176098	1	1.000000										
87	1	1	1	9	8	0.185302	0.286673	82.043	4.2	3.5	0.640	1171.2125
1.173593	1	1.000000										
88	1	0	0	10	2	0.186016	0.285734	82.281	5.4	6.1	0.896	6057.2881
1.170806	1	1.000000										
89	1	0	2	8	4	0.186795	0.284717	82.538	0.5	0.5	0.096	259.0858
1.167808	1	1.000000										
90	1	1	3	3	8	0.186855	0.284639	82.558	12.8	14.2	1.701	3602.4695
1.167578	1	1.000000										
91	1	3	0	4	4	0.186884	0.284601	82.567	3.4	3.7	0.354	1933.2856
1.167467	1	1.000000										
92	1	2	0	8	4	0.188440	0.282595	83.075	0.4	0.7	0.450	254.6404
1.161619	1	1.000000										
93	1	3	1	3	8	0.190173	0.280397	83.631	12.4	13.5	1.625	3544.1260

											ZTm123	
1.155305		1.000000										
94	1	0 3	5	4	0.197387	0.271624	85.850	0.2	0.0	0.269	101.9268	
1.131032		1.000000										
95	1	1 3	4	8	0.198052	0.270844	86.048	2.0	0.0	0.787	585.4951	
1.128943		1.000000										
96	1	0 1	10	4	0.200727	0.267750	86.830	10.5	19.1	15.456	6287.6836	
1.120768		1.000000										
97	1	1 0	10	4	0.201189	0.267223	86.964	10.1	15.0	7.168	6052.9536	
1.119392		1.000000										
98	1	3 0	5	4	0.201492	0.266878	87.051	0.2	0.2	0.073	96.8589	
1.118493		1.000000										
99	1	3 1	4	8	0.201714	0.266626	87.115	1.9	2.4	0.585	574.5877	
1.117838		1.000000										
100	1	1 2	8	8	0.202078	0.266214	87.219	13.7	15.6	2.219	4113.2598	
1.116771		1.000000										
101	1	2 2	6	8	0.202410	0.265839	87.314	25.3	27.3	2.377	7587.8877	
1.115802		1.000000										
102	1	2 1	8	8	0.203484	0.264633	87.619	10.9	8.4	1.984	3283.2864	
1.112702		1.000000										
103	1	1 3	5	8	0.214163	0.253185	90.515	4.4	2.2	1.532	1360.9369	
1.084481		1.000000										
104	1	0 2	9	4	0.216006	0.251302	90.991	3.2	4.7	2.185	2001.0729	
1.080040		1.000000										
105	1	0 3	6	4	0.217252	0.250042	91.310	2.7	4.2	2.266	1683.4269	
1.077099		1.000000										
106	1	1 1	10	8	0.217973	0.249319	91.493	8.9	9.8	1.196	2771.9487	
1.075422		1.000000										
107	1	2 0	9	4	0.218095	0.249196	91.524	3.2	3.3	0.219	1981.4745	
1.075139		1.000000										
108	1	3 1	5	8	0.218318	0.248974	91.580	4.3	4.1	0.360	1347.4934	
1.074625		1.000000										
109	1	2 3	0	4	0.220382	0.246927	92.098	3.3	2.6	0.892	2071.3640	
1.069933		1.000000										
110	1	3 0	6	4	0.222043	0.245302	92.509	2.1	1.6	0.581	1313.8370	
1.066253		1.000000										
111	1	2 3	1	8	0.222390	0.244965	92.594	0.1	0.1	0.029	38.9376	
1.065494		1.000000										
112	1	0 0	11	2	0.222907	0.244464	92.721	2.0	2.0	0.299	2481.0325	
1.064369		1.000000										
113	1	3 2	0	4	0.223083	0.244293	92.764	3.0	3.1	0.482	1859.6876	
1.063987		1.000000										
114	1	3 2	1	8	0.225130	0.242330	93.261	0.2	0.0	0.240	76.5864	
1.059620		1.000000										

115	1	2	2	7	8	0.227237	0.240336	ZTm123 93.765	8.4	11.0	3.594	2648.5308
1.055242		1.000000										
116	1	2	3	2	8	0.228587	0.239073	94.085	1.3	1.6	0.417	400.5310
1.052499		1.000000										
117	1	3	2	2	8	0.231448	0.236433	94.753	1.4	2.5	2.166	448.1478
1.046837		1.000000										
118	1	1	2	9	8	0.235426	0.232842	95.661	7.3	6.2	1.363	2339.5327
1.039286		1.000000										
119	1	1	3	6	8	0.236853	0.231575	95.982	25.9	24.5	1.627	8271.8154
1.036665		1.000000										
120	1	2	1	9	8	0.237216	0.231254	96.063	7.2	5.7	1.232	2306.6516
1.036004		1.000000										

No. d-hkl	Code	H	K	L	Mult	Hw	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2
		CORR										
121	1	2	3	3	8	0.239533	0.229226	96.576	29.6	30.4	1.353	9452.0215
1.031859		1.000000										
122	1	3	1	6	8	0.241720	0.227337	97.054	25.4	27.1	1.897	8126.2109
1.028046		1.000000										
123	1	3	2	3	8	0.242611	0.226575	97.246	31.5	31.7	0.857	10087.8838
1.026521		1.000000										
124	1	0	1	11	4	0.242707	0.226493	97.267	0.2	0.2	0.006	123.6940
1.026357		1.000000										
125	1	1	0	11	4	0.243331	0.225962	97.401	0.4	0.4	0.044	261.3219
1.025300		1.000000										
126	1	0	3	7	4	0.245108	0.224459	97.782	3.1	2.2	0.816	2007.8640
1.022326		1.000000										
127	1	3	0	7	4	0.250899	0.219671	98.993	2.9	2.7	0.987	1856.1964
1.013038		1.000000										
128	1	2	3	4	8	0.256290	0.215353	100.085	4.5	7.3	4.870	1425.0371
1.004901		1.000000										
129	1	0	2	10	4	0.258244	0.213819	100.473	7.2	7.8	1.008	4574.9458
1.002065		1.000000										
130	1	3	2	4	8	0.259713	0.212677	100.762	4.1	4.7	0.779	1324.2474
0.999970		1.000000										
131	1	2	0	10	4	0.261010	0.211676	101.015	7.1	6.4	0.893	4540.1323
0.998147		1.000000										
132	1	2	2	8	8	0.262351	0.210649	101.275	0.5	0.4	0.114	155.3315
0.996288		1.000000										
133	1	1	1	11	8	0.266121	0.207799	101.996	9.4	7.6	1.774	2983.8374
0.991193		1.000000										
134	1	1	3	7	8	0.268898	0.205736	102.518	8.9	8.6	0.873	2831.3657

ZTm123											
0.987560		1.000000									
135	1	3 1	7	8	0.274850	0.201414	103.612	8.8	10.6	2.547	2781.7654
0.980101		1.000000									
136	1	0 0	12	2	0.278553	0.198790	104.275	0.4	0.0	0.349	480.5932
0.975671		1.000000									
137	1	2 3	5	8	0.280712	0.197282	104.657	0.3	0.1	0.338	108.8133
0.973158		1.000000									
138	1	1 2	10	8	0.284149	0.194915	105.255	14.4	20.4	8.553	4516.4150
0.969261		1.000000									
139	1	0 4	0	2	0.284582	0.194620	105.330	10.9	13.8	3.666	13684.8662
0.968778		1.000000									
140	1	3 2	5	8	0.284673	0.194558	105.346	0.3	0.4	0.095	96.7802
0.968677		1.000000									
141	1	0 3	8	4	0.284882	0.194416	105.382	4.2	5.1	1.115	2617.9429
0.968446		1.000000									
142	1	2 1	10	8	0.286562	0.193277	105.670	14.8	14.7	0.596	4643.6846
0.966597		1.000000									
143	1	0 4	1	4	0.287591	0.192584	105.845	0.1	0.1	0.013	91.9060
0.965479		1.000000									
144	1	3 0	8	4	0.292254	0.189487	106.629	5.1	3.7	1.427	3159.7217
0.960539		1.000000									
145	1	0 4	2	4	0.296937	0.186445	107.398	0.1	0.1	0.021	49.8809
0.955779		1.000000									
146	1	4 0	0	2	0.297884	0.185838	107.552	10.7	9.8	1.435	13241.8389
0.954840		1.000000									
147	1	4 0	1	4	0.301128	0.183779	108.073	0.1	0.2	0.081	85.9974
0.951681		1.000000									
148	1	0 1	12	4	0.307039	0.180104	109.002	0.4	0.7	0.802	220.5076
0.946143		1.000000									
149	1	1 0	12	4	0.307949	0.179548	109.143	0.6	0.8	0.637	338.3168
0.945315		1.000000									
150	1	4 0	2	4	0.311222	0.177563	109.645	0.1	0.0	0.089	50.0887
0.942387		1.000000									
151	1	0 4	3	4	0.313676	0.176094	110.017	3.0	3.5	0.736	1800.2323
0.940243		1.000000									
152	1	2 2	9	8	0.313836	0.175999	110.041	4.8	5.3	0.861	1456.0321
0.940104		1.000000									
153	1	1 4	0	4	0.315072	0.175265	110.226	2.6	2.5	0.283	1571.2277
0.939041		1.000000									
154	1	1 3	8	8	0.315427	0.175056	110.279	0.4	0.4	0.041	112.3651
0.938739		1.000000									
155	1	2 3	6	8	0.316104	0.174656	110.380	4.4	4.0	0.560	1325.5385
0.938163		1.000000									

								ZTm123				
156	1	1	4	1	8	0.318637	0.173172	110.756	0.2	0.2	0.050	49.8939
0.936035		1.000000										
157	1	3	2	6	8	0.320931	0.171842	111.092	3.5	4.8	1.893	1059.7568
0.934146		1.000000										
158	1	0	2	11	4	0.322494	0.170944	111.320	3.3	4.2	1.221	1976.7295
0.932879		1.000000										
159	1	3	1	8	8	0.323183	0.170550	111.419	0.4	0.5	0.122	112.7497
0.932325		1.000000										
160	1	2	0	11	4	0.326481	0.168679	111.892	3.3	2.3	0.956	1964.2559
0.929715		1.000000										
161	1	4	0	3	4	0.329368	0.167063	112.301	3.0	2.3	0.667	1758.1469
0.927484		1.000000										
162	1	1	4	2	8	0.329756	0.166848	112.356	1.4	1.0	0.309	404.3893
0.927188		1.000000										
163	1	4	1	0	4	0.329858	0.166791	112.370	2.9	2.2	0.646	1688.0527
0.927110		1.000000										
164	1	4	1	1	8	0.333716	0.164666	112.908	0.1	0.1	0.090	23.4571
0.924217		1.000000										
165	1	0	4	4	4	0.339958	0.161301	113.759	0.2	0.7	2.322	88.2068
0.919712		1.000000										
166	1	1	1	12	8	0.341854	0.160295	114.013	1.0	2.3	3.032	282.5061
0.918384		1.000000										
167	1	0	3	9	4	0.344437	0.158938	114.357	3.0	1.8	1.050	1760.3254
0.916605		1.000000										
168	1	4	1	2	8	0.345773	0.158241	114.533	1.3	0.6	0.421	361.0078
0.915698		1.000000										
169	1	1	4	3	8	0.349850	0.156139	115.065	27.3	26.5	1.580	7799.7139
0.912984		1.000000										
170	1	3	0	9	4	0.354646	0.153710	115.679	3.1	0.8	0.714	1742.5491
0.909893		1.000000										
171	1	4	0	4	4	0.358052	0.152013	116.109	0.2	0.2	0.032	85.8126
0.907761		1.000000										
172	1	3	3	0	4	0.359726	0.151187	116.317	14.9	17.8	3.656	8386.5029
0.906731		1.000000										
173	1	1	2	11	8	0.360536	0.150790	116.418	0.6	0.5	0.054	161.6216
0.906238		1.000000										
174	1	2	1	11	8	0.364165	0.149023	116.865	0.3	0.4	0.087	83.8987
0.904059		1.000000										
175	1	3	3	1	8	0.364225	0.148994	116.872	0.0	0.0	0.008	7.8654
0.904024		1.000000										
176	1	4	1	3	8	0.367669	0.147341	117.290	25.4	30.1	5.754	7044.6968
0.902008		1.000000										
177	1	2	3	7	8	0.368896	0.146757	117.438	5.6	6.1	0.623	1556.4579

No.	Code	H	K	L	Mult	HW	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2
0.901301	1	0	0	13	2	0.370088	0.146193	117.581	2.4	2.5	0.135	2682.0103
0.900620	1	3	2	7	8	0.375243	0.143782	118.191	5.3	2.8	1.503	1455.0631
0.897738	1	3	3	2	8	0.378352	0.142350	118.553	0.4	0.4	0.079	118.2243
0.896046	1	0	0	13	2	0.370088	0.146193	117.581	2.4	2.5	0.135	2682.0103
0.895190	1	1	4	4	8	0.381912	0.140731	118.963	3.5	3.0	0.673	962.3867
0.894153	1	1	3	9	8	0.387443	0.138258	119.588	2.4	3.2	1.262	661.7478

 BRAGG R-Factors and weight fractions for Pattern # 1

=> Phase: 1 ZTm123
 => Bragg R-factor: 8.94 Vol: 173.285(0.000) Fract(%): 100.00(0.00)
 => Rf-factor= 9.62 ATZ: 743.323 Brindley: 1.0000

CPU Time: 0.812 seconds
 0.014 minutes

=> Run finished at: Date: 24/12/2017 Time: 11:40:51.558