

ZY123

** 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: 12/12/2017 Time: 09:44:29.573

=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 8.11
=> RF-factor : 7.69

Pattern# 1 Phase No: 1 Phase name: ZY123

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	0.133358	0.605541	22.748	62.0	76.2	18.440	1949.2006
3.905870		1.000000										
2	1	0	1	0	2	0.133549	0.604794	22.847	74.8	80.6	9.309	2372.6780
3.889061		1.000000										
3	1	1	0	0	2	0.134251	0.602034	23.216	46.2	54.9	10.294	1516.2616
3.828227		1.000000										
4	1	0	1	1	4	0.135911	0.595468	24.091	4.5	7.2	4.336	79.5484
3.691072		1.000000										
5	1	1	0	1	4	0.136572	0.592840	24.441	1.9	5.9	12.923	33.8403
3.638944		1.000000										
6	1	0	1	2	4	0.142262	0.569863	27.505	53.0	61.0	9.161	1239.5957
3.240179		1.000000										
7	1	1	0	2	4	0.142830	0.567537	27.815	74.2	88.4	16.809	1777.1595
3.204744		1.000000										
8	1	0	0	4	2	0.147675	0.547474	30.490	8.0	10.6	3.496	462.9867
2.929403		1.000000										
9	1	0	1	3	4	0.151190	0.532693	32.461	740.0	713.8	25.170	24609.1602

ZY123											
2.755905		1.000000									
10	1	1 0	3	4	0.151663	0.530688	32.728	828.4	800.8	26.533	28035.7578
2.734003		1.000000									
11	1	1 1	0	4	0.151789	0.530153	32.800	808.9	786.4	21.739	27503.7520
2.728219		1.000000									
12	1	1 1	1	8	0.153383	0.523380	33.703	18.3	24.3	7.948	329.7188
2.657147		1.000000									
13	1	1 1	2	8	0.157912	0.503952	36.293	44.7	57.1	15.770	945.4064
2.473218		1.000000									
14	1	0 0	5	2	0.161519	0.488316	38.378	101.7	113.6	13.276	9709.6895
2.343522		1.000000									
15	1	0 1	4	4	0.161626	0.487849	38.440	64.1	70.1	6.490	3072.4067
2.339876		1.000000									
16	1	1 0	4	4	0.162023	0.486117	38.671	47.2	57.4	12.356	2290.5469
2.326427		1.000000									
17	1	1 1	3	8	0.164800	0.473978	40.290	231.4	241.7	10.941	6145.6509
2.236628		1.000000									
18	1	0 1	5	4	0.173033	0.437659	45.132	6.9	8.8	2.576	468.7185
2.007254		1.000000									
19	1	1 0	5	4	0.173376	0.436138	45.335	4.9	6.3	1.700	341.1454
1.998744		1.000000									
20	1	1 1	4	8	0.173468	0.435731	45.389	8.9	12.1	4.384	307.5006
1.996480		1.000000									
21	1	0 0	6	2	0.175277	0.427701	46.460	135.0	161.9	32.053	19648.6504
1.952935		1.000000									
22	1	0 2	0	2	0.175635	0.426106	46.672	256.6	253.4	3.686	37735.3711
1.944530		1.000000									
23	1	0 2	1	4	0.176777	0.421029	47.349	0.8	1.0	0.268	58.4602
1.918296		1.000000									
24	1	2 0	0	2	0.176962	0.420206	47.459	242.7	236.6	6.190	37036.2617
1.914114		1.000000									
25	1	2 0	1	4	0.178089	0.415192	48.128	0.7	0.7	0.112	57.1625
1.889075		1.000000									
26	1	0 2	2	4	0.180127	0.406116	49.338	4.0	5.6	2.423	329.6037
1.845536		1.000000									
27	1	2 0	2	4	0.181398	0.400453	50.093	3.8	4.9	1.607	326.3032
1.819472		1.000000									
28	1	1 1	5	8	0.183520	0.390993	51.354	56.7	65.8	10.524	2579.7959
1.777708		1.000000									
29	1	0 1	6	4	0.185249	0.383291	52.381	13.7	15.0	1.645	1298.7698
1.745247		1.000000									
30	1	0 2	3	4	0.185495	0.382195	52.527	15.3	17.8	2.936	1463.5925
1.740737		1.000000									

31	1	1	0	6	4	0.185554	0.381929	ZY123 52.563	7.6	8.9	1.470	728.9643
1.739645		1.000000										
32	1	1	2	0	4	0.185881	0.380472	52.757	13.6	15.0	1.629	1311.4321
1.733696		1.000000										
33	1	2	0	3	4	0.186711	0.376778	53.250	14.8	16.2	1.610	1456.0217
1.718814		1.000000										
34	1	2	1	0	4	0.186792	0.376417	53.298	17.2	18.6	1.552	1703.1006
1.717374		1.000000										
35	1	1	2	1	8	0.186924	0.375826	53.377	0.4	0.4	0.036	19.7154
1.715026		1.000000										
36	1	2	1	1	8	0.187828	0.371803	53.913	1.0	0.0	0.367	52.1005
1.699221		1.000000										
37	1	0	0	7	2	0.189314	0.365190	54.795	21.1	26.2	6.351	4441.4849
1.673944		1.000000										
38	1	1	2	2	8	0.190008	0.362104	55.206	20.5	21.3	1.211	1094.7828
1.662438		1.000000										
39	1	2	1	2	8	0.190892	0.358171	55.731	15.5	15.7	0.847	846.3981
1.648031		1.000000										
40	1	0	2	4	4	0.192662	0.350315	56.778	0.8	0.0	0.221	89.4320
1.620089		1.000000										
41	1	2	0	4	4	0.193822	0.345171	57.464	0.7	0.6	0.148	85.4480
1.602372		1.000000										
42	1	1	1	6	8	0.194785	0.340904	58.033	239.4	267.5	31.293	14275.0146
1.588010		1.000000										
43	1	1	2	3	8	0.195016	0.339881	58.169	290.0	304.0	14.680	17384.9941
1.584610		1.000000										
44	1	2	1	3	8	0.195876	0.336077	58.676	255.3	264.4	9.665	15596.3252
1.572118		1.000000										
45	1	0	1	7	4	0.198343	0.325183	60.129	9.7	12.0	2.960	1248.4774
1.537565		1.000000										
46	1	1	0	7	4	0.198626	0.323939	60.295	10.5	13.2	3.294	1366.6021
1.533730		1.000000										
47	1	0	2	5	4	0.201465	0.311456	61.959	40.0	41.6	2.087	5493.9399
1.496466		1.000000										
48	1	1	2	4	8	0.201819	0.309906	62.166	19.4	22.0	2.914	1345.1974
1.491986		1.000000										
49	1	2	0	5	4	0.202579	0.306576	62.610	38.5	41.4	3.229	5414.8203
1.482469		1.000000										
50	1	2	1	4	8	0.202653	0.306250	62.653	23.9	25.0	1.228	1684.3173
1.481545		1.000000										
51	1	0	0	8	2	0.204033	0.300222	63.457	0.7	1.2	0.815	212.6671
1.464701		1.000000										
52	1	1	1	7	8	0.207295	0.286027	65.350	30.7	39.9	11.903	2364.4150

ZY123												
1.426785		1.000000										
53	1	1 2	5	8	0.210333	0.272902	67.100	3.8	2.9	0.986	307.6491	
1.393763		1.000000										
54	1	2 1	5	8	0.211149	0.269391	67.568	4.6	2.3	1.273	382.1238	
1.385240		1.000000										
55	1	0 2	6	4	0.211858	0.266347	67.974	74.6	87.3	14.745	12453.5840	
1.377953		1.000000										
56	1	0 1	8	4	0.212573	0.263282	68.382	29.9	40.0	13.531	5043.3555	
1.370711		1.000000										
57	1	1 0	8	4	0.212845	0.262121	68.537	33.6	38.3	5.421	5694.5986	
1.367992		1.000000										
58	1	2 0	6	4	0.212944	0.261696	68.594	72.4	79.1	7.355	12298.6006	
1.367002		1.000000										
59	1	2 2	0	4	0.213235	0.260453	68.760	133.9	146.7	13.973	22862.5723	
1.364110		1.000000										
60	1	2 2	1	8	0.214167	0.256476	69.290	0.4	0.2	0.113	32.1051	
1.354959		1.000000										

No. d-hkl	Code	H CORR	K	L	Mult	Hw	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2
61	1	2 2	2	8	0.216958	0.244624	70.870	2.8	4.2	2.209	258.0881	
1.328574		1.000000										
62	1	0 0	9	2	0.219944	0.232056	72.546	3.7	5.0	2.015	1399.0215	
1.301957		1.000000										
63	1	1 2	6	8	0.220577	0.229409	72.899	7.5	10.6	4.394	714.8541	
1.296521		1.000000										
64	1	0 3	0	2	0.220596	0.229327	72.910	3.9	5.6	2.421	1497.9684	
1.296354		1.000000										
65	1	1 1	8	8	0.221289	0.226435	73.295	7.5	8.3	0.948	720.2324	
1.290483		1.000000										
66	1	2 1	6	8	0.221387	0.226023	73.350	11.2	11.4	0.460	1085.3464	
1.289652		1.000000										
67	1	0 3	1	4	0.221526	0.225447	73.427	0.2	0.2	0.014	40.0968	
1.288492		1.000000										
68	1	2 2	3	8	0.221605	0.225116	73.471	13.3	12.5	0.910	1293.6395	
1.287829		1.000000										
69	1	3 0	0	2	0.223030	0.219193	74.261	3.1	4.4	1.990	1227.8851	
1.276076		1.000000										
70	1	0 2	7	4	0.223954	0.215367	74.771	15.0	14.1	1.273	3003.5288	
1.268628		1.000000										
71	1	3 0	1	4	0.223960	0.215339	74.775	0.1	0.1	0.008	18.0452	
1.268576		1.000000										

72	1	0	3	2	4	0.224317	0.213867	ZY123 74.971	3.2	3.3	0.244	647.5397
1.265739	1	1.000000										
73	1	2	0	7	4	0.225037	0.210896	75.367	14.6	15.0	0.992	2970.2678
1.260067	1	1.000000										
74	1	3	0	2	4	0.226758	0.203833	76.309	3.8	3.4	0.891	777.5118
1.246844	1	1.000000										
75	1	2	2	4	8	0.228130	0.198230	77.056	0.2	0.4	0.485	21.8165
1.236609	1	1.000000										
76	1	0	1	9	4	0.228403	0.197122	77.204	17.5	23.2	7.445	3705.0364
1.234610	1	1.000000										
77	1	1	0	9	4	0.228675	0.196014	77.351	21.1	26.0	5.989	4477.9160
1.232622	1	1.000000										
78	1	0	3	3	4	0.228987	0.194747	77.520	52.2	59.0	7.750	11090.9580
1.230358	1	1.000000										
79	1	1	3	0	4	0.229333	0.193345	77.707	58.0	61.7	4.030	12376.7803
1.227864	1	1.000000										
80	1	1	3	1	8	0.230271	0.189548	78.214	0.7	0.3	0.246	77.5063
1.221178	1	1.000000										
81	1	3	0	3	4	0.231445	0.184817	78.844	54.0	54.3	0.994	11796.8691
1.212981	1	1.000000										
82	1	3	1	0	4	0.231519	0.184521	78.884	55.5	55.5	0.858	12124.1270
1.212475	1	1.000000										
83	1	3	1	1	8	0.232462	0.180740	79.388	0.7	0.9	0.319	75.7991
1.206036	1	1.000000										
84	1	1	2	7	8	0.232730	0.179668	79.531	9.2	8.8	0.782	1014.7902
1.204227	1	1.000000										
85	1	1	3	2	8	0.233098	0.178196	79.727	3.6	3.3	0.368	395.1180
1.201756	1	1.000000										
86	1	2	1	7	8	0.233554	0.176375	79.970	8.4	7.5	1.014	932.9418
1.198717	1	1.000000										
87	1	3	1	2	8	0.235303	0.169431	80.896	3.4	3.1	0.716	388.5476
1.187316	1	1.000000										
88	1	0	3	4	4	0.235593	0.168284	81.049	4.9	4.7	0.595	1113.2180
1.185463	1	1.000000										
89	1	2	2	5	8	0.236627	0.164207	81.592	31.8	34.0	2.594	3657.8215
1.178933	1	1.000000										
90	1	1	1	9	8	0.237257	0.161731	81.923	4.8	6.0	1.448	556.1036
1.175016	1	1.000000										
91	1	0	0	10	2	0.237786	0.159657	82.199	4.3	5.7	1.839	1997.7280
1.171761	1	1.000000										
92	1	1	3	3	8	0.237854	0.159392	82.234	23.9	30.7	8.669	2779.4028
1.171348	1	1.000000										
93	1	0	2	8	4	0.238085	0.158488	82.355	0.6	0.7	0.063	149.8106

ZY123											
1.169938		1.000000									
94	1	3 0	4	4	0.238092	0.158461	82.359	3.8	4.1	0.352	874.3643
1.169897		1.000000									
95	1	2 0	8	4	0.239202	0.154132	82.936	0.6	0.0	0.407	148.8623
1.163213		1.000000									
96	1	3 1	3	8	0.240090	0.150684	83.396	23.2	26.6	4.172	2738.9080
1.157966		1.000000									
97	1	0 3	5	4	0.244275	0.134620	85.537	1.4	3.1	3.786	341.2647
1.134367		1.000000									
98	1	1 3	4	8	0.244636	0.133247	85.720	1.2	0.0	0.423	151.7734
1.132411		1.000000									
99	1	0 1	10	4	0.246615	0.125775	86.717	19.8	29.3	13.991	4901.6484
1.121942		1.000000									
100	1	3 0	5	4	0.246854	0.124878	86.836	1.1	1.4	0.328	284.8909
1.120705		1.000000									
101	1	1 0	10	4	0.246903	0.124693	86.861	20.1	24.0	4.674	4978.7334
1.120450		1.000000									
102	1	3 1	4	8	0.246931	0.124588	86.875	1.2	1.4	0.252	149.8725
1.120306		1.000000									
103	1	1 2	8	8	0.247212	0.123533	87.016	32.4	36.7	4.840	4025.9597
1.118856		1.000000									
104	1	2 2	6	8	0.247318	0.123138	87.068	69.7	79.8	11.604	8658.5420
1.118314		1.000000									
105	1	2 1	8	8	0.248079	0.120289	87.448	28.6	28.6	0.755	3573.1597
1.114432		1.000000									
106	1	1 3	5	8	0.253649	0.099791	90.181	11.5	12.8	1.863	1479.8291
1.087623		1.000000									
107	1	0 2	9	4	0.254923	0.095181	90.796	4.2	6.2	3.127	1077.6471
1.081853		1.000000									
108	1	0 3	6	4	0.255326	0.093733	90.989	3.7	3.7	0.480	960.4398
1.080060		1.000000									
109	1	3 1	5	8	0.256045	0.091150	91.333	11.3	12.3	1.207	1455.4653
1.076884		1.000000									
110	1	1 1	10	8	0.256097	0.090965	91.358	10.2	11.0	0.893	1323.9313
1.076657		1.000000									
111	1	2 0	9	4	0.256126	0.090860	91.372	4.1	4.4	0.319	1069.9373
1.076529		1.000000									
112	1	2 3	0	4	0.256855	0.088253	91.720	5.2	4.9	0.507	1347.8654
1.073354		1.000000									
113	1	2 3	1	8	0.257900	0.084537	92.215	0.2	0.2	0.056	31.1333
1.068879		1.000000									
114	1	3 0	6	4	0.258049	0.084008	92.286	2.6	2.4	0.523	678.1794
1.068248		1.000000									

115	1	3	2	0	4	0.258376	0.082849	ZY123 92.440	4.4	4.9	0.772	1147.9381
1.066866		1.000000										
116	1	0	0	11	2	0.258764	0.081477	92.623	9.0	9.6	0.965	4683.4736
1.065237		1.000000										
117	1	3	2	1	8	0.259429	0.079131	92.936	0.1	0.2	0.042	16.5983
1.062471		1.000000										
118	1	2	2	7	8	0.260656	0.074830	93.509	16.5	20.7	5.377	2159.6870
1.057458		1.000000										
119	1	2	3	2	8	0.261071	0.073380	93.703	3.8	4.7	1.132	502.8378
1.055783		1.000000										
120	1	3	2	2	8	0.262630	0.067966	94.425	4.5	1.6	1.444	595.5590
1.049606		1.000000										

No. d-hkl	Code	H	K	L	Mult	Hw	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2
		CORR										
121	1	1	2	9	8	0.264854	0.060325	95.443	24.9	31.9	8.975	3291.9060
1.041080		1.000000										
122	1	1	3	6	8	0.265280	0.058870	95.637	53.5	58.0	5.042	7066.8916
1.039481		1.000000										
123	1	2	1	9	8	0.265810	0.057069	95.877	20.7	19.1	1.527	2740.8713
1.037513		1.000000										
124	1	2	3	3	8	0.266497	0.054739	96.188	61.4	54.0	6.581	8123.4790
1.034986		1.000000										
125	1	3	1	6	8	0.267850	0.050179	96.796	52.3	50.5	1.993	6935.6162
1.030095		1.000000										
126	1	3	2	3	8	0.268111	0.049304	96.913	65.5	64.8	1.309	8688.6738
1.029165		1.000000										
127	1	0	1	11	4	0.268610	0.047631	97.136	0.6	0.6	0.017	153.7225
1.027394		1.000000										
128	1	1	0	11	4	0.268936	0.046542	97.281	0.4	0.5	0.140	114.9528
1.026248		1.000000										
129	1	0	3	7	4	0.269311	0.045295	97.447	2.9	4.1	1.730	760.5159
1.024940		1.000000										
130	1	3	0	7	4	0.272285	0.035477	98.756	3.0	7.0	9.204	803.9237
1.014830		1.000000										
131	1	2	3	4	8	0.274435	0.028486	99.688	5.9	10.4	8.246	778.9756
1.007832		1.000000										
132	1	0	2	10	4	0.275766	0.024206	100.259	6.1	8.6	3.521	1627.2671
1.003627		1.000000										
133	1	3	2	4	8	0.276142	0.023002	100.420	4.7	6.1	1.930	626.5400
1.002455		1.000000										
134	1	2	0	10	4	0.277142	0.019812	100.845	6.1	4.1	1.533	1617.1521

ZY123											
0.999372		1.000000									
135	1	2 2	8	8	0.277514	0.018632	101.002	1.0	0.4	0.305	131.6734
0.998240		1.000000									
136	1	1 1	11	8	0.279509	0.012343	101.841	19.1	26.7	10.793	2524.5144
0.992281		1.000000									
137	1	1 3	7	8	0.280266	0.009975	102.157	10.1	10.3	0.617	1331.7538
0.990070		1.000000									
138	1	3 1	7	8	0.283132	0.001116	103.338	10.0	12.8	3.980	1309.4252
0.981949		1.000000									
139	1	0 0	12	2	0.285144	-0.005013	104.155	1.3	0.6	0.599	665.1813
0.976468		1.000000									
140	1	2 3	5	8	0.285368	-0.005691	104.245	2.3	1.2	0.964	302.9030
0.975869		1.000000									
141	1	0 4	0	2	0.286733	-0.009798	104.793	22.6	21.4	1.574	11798.9414
0.972265		1.000000									
142	1	3 2	5	8	0.287226	-0.011271	104.990	2.0	2.0	0.062	259.8170
0.970985		1.000000									
143	1	1 2	10	8	0.287290	-0.011463	105.015	28.7	29.8	1.379	3747.1021
0.970819		1.000000									
144	1	0 3	8	4	0.287317	-0.011544	105.026	10.3	10.8	0.589	2692.1343
0.970749		1.000000									
145	1	0 4	1	4	0.288022	-0.013644	105.306	0.1	0.1	0.005	17.7680
0.968935		1.000000									
146	1	2 1	10	8	0.288418	-0.014821	105.463	28.1	27.6	1.057	3660.4285
0.967925		1.000000									
147	1	3 0	8	4	0.290736	-0.021641	106.372	11.3	9.0	2.284	2933.9138
0.962146		1.000000									
148	1	0 4	2	4	0.291972	-0.025240	106.852	0.7	0.9	0.299	183.3253
0.959148		1.000000									
149	1	4 0	0	2	0.292849	-0.027776	107.190	22.1	29.9	10.721	11382.9404
0.957057		1.000000									
150	1	4 0	1	4	0.294206	-0.031669	107.709	0.1	0.0	0.347	17.3545
0.953880		1.000000									
151	1	0 1	12	4	0.297215	-0.040186	108.845	0.5	7.1	92.425	128.2133
0.947071		1.000000									
152	1	1 0	12	4	0.297623	-0.041328	108.997	0.3	2.0	9.275	87.4992
0.946173		1.000000									
153	1	4 0	2	4	0.298372	-0.043417	109.276	0.7	2.7	7.444	179.4712
0.944538		1.000000									
154	1	0 4	3	4	0.298864	-0.044784	109.458	4.2	5.7	2.225	1060.1238
0.943474		1.000000									
155	1	1 4	0	4	0.299390	-0.046237	109.652	4.2	4.2	0.416	1054.2681
0.942348		1.000000									

							ZY123					
156	1	2	2	9	8	0.299633	-0.046911	109.741	6.9	6.8	0.583	874.1460
0.941829		1.000000										
157	1	1	3	8	8	0.300040	-0.048030	109.891	4.1	3.5	0.537	509.6794
0.940967		1.000000										
158	1	2	3	6	8	0.300192	-0.048450	109.947	6.7	5.4	1.146	844.6479
0.940645		1.000000										
159	1	1	4	1	8	0.300826	-0.050188	110.178	0.1	0.1	0.014	15.1667
0.939316		1.000000										
160	1	3	2	6	8	0.302301	-0.054209	110.715	5.0	7.1	3.203	623.0983
0.936269		1.000000										
161	1	0	2	11	4	0.303303	-0.056916	111.076	13.9	13.5	1.046	3459.1750
0.934240		1.000000										
162	1	3	1	8	8	0.303429	-0.057255	111.121	4.1	4.0	0.286	505.2928
0.933987		1.000000										
163	1	2	0	11	4	0.305035	-0.061556	111.694	13.9	12.1	1.742	3427.9924
0.930805		1.000000										
164	1	1	4	2	8	0.305247	-0.062120	111.769	3.9	3.8	0.245	475.8210
0.930390		1.000000										
165	1	4	0	3	4	0.305676	-0.063257	111.921	4.2	4.8	0.682	1044.6685
0.929558		1.000000										
166	1	4	1	0	4	0.305793	-0.063569	111.963	4.9	5.5	0.794	1194.1517
0.929330		1.000000										
167	1	4	1	1	8	0.307315	-0.067581	112.498	0.2	0.0	0.937	24.3206
0.926421		1.000000										
168	1	0	4	4	4	0.309277	-0.072696	113.179	0.0	0.0	0.038	1.4196
0.922768		1.000000										
169	1	1	1	12	8	0.311164	-0.077553	113.827	10.4	9.5	2.378	1249.6105
0.919356		1.000000										
170	1	0	3	9	4	0.311570	-0.078589	113.965	8.8	9.7	1.159	2121.1814
0.918635		1.000000										
171	1	4	1	2	8	0.312012	-0.079714	114.115	3.3	4.0	0.910	391.8179
0.917855		1.000000										
172	1	1	4	3	8	0.313037	-0.082313	114.462	56.4	56.6	1.786	6734.1128
0.916064		1.000000										
173	1	3	0	9	4	0.315824	-0.089286	115.391	10.5	9.0	1.740	2469.1755
0.911334		1.000000										
174	1	4	0	4	4	0.316793	-0.091680	115.711	0.0	0.0	0.001	1.2153
0.909736		1.000000										
175	1	3	3	0	4	0.316994	-0.092176	115.777	29.3	34.0	5.653	6859.9766
0.909406		1.000000										
176	1	1	2	11	8	0.318107	-0.094902	116.140	0.9	1.1	0.257	108.7520
0.907604		1.000000										
177	1	3	3	1	8	0.318684	-0.096309	116.328	0.4	0.4	0.052	47.0210

ZY123													
No.	Code	H	K	L	Mult	HW	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2	
d-hkl		CORR											
0.906680	1	1.000000	2	1	11	8	0.319596	-0.098518	116.622	1.3	1.0	0.306	152.5253
0.905238	1	1.000000	4	1	3	8	0.320329	-0.100287	116.858	52.4	42.0	8.509	6049.7373
0.904092	1	1.000000	2	3	7	8	0.320673	-0.101114	116.968	5.5	4.7	0.671	630.7682
0.903558	1	1.000000											
0.901355	1	1.000000	0	0	13	2	0.322113	-0.104551	117.427	5.3	7.1	2.418	2412.7659
0.899677	1	1.000000	3	2	7	8	0.323229	-0.107195	117.779	5.9	7.4	2.076	668.3497
0.898645	1	1.000000	3	3	2	8	0.323925	-0.108833	117.998	2.2	2.2	0.204	251.2029
0.898046	1	1.000000	0	4	5	4	0.324333	-0.109787	118.125	9.1	7.0	1.746	2050.9038
0.897075	1	1.000000	1	4	4	8	0.324998	-0.111342	118.332	4.2	3.5	0.773	477.3654
0.893277	1	1.000000	1	3	9	8	0.327665	-0.117502	119.154	3.8	9.4	13.846	424.0608

 BRAGG R-Factors and weight fractions for Pattern # 1

=> Phase: 1 ZY123
 => Bragg R-factor: 8.11 Vol: 174.454(0.000) Fract(%): 100.00(0.00)
 => Rf-factor= 7.69 ATZ: 663.294 Brindley: 1.0000

CPU Time: 1.500 seconds
 0.025 minutes

=> Run finished at: Date: 12/12/2017 Time: 09:44:31.135