

ZNd123

** 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: 09:46:03.826

=> -----> Pattern# 1
=> Phase: 1
=> Bragg R-factor: 8.30
=> RF-factor : 8.64

Pattern# 1 Phase No: 1 Phase name: ZNd123

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	0.219102	0.608805	22.644	22.9	24.2	1.470	3056.3706
3.923602		1.000000										
2	1	0	1	0	2	0.219101	0.608764	22.663	35.5	37.6	2.404	4740.8540
3.920311		1.000000										
3	1	1	0	0	2	0.219099	0.608281	22.892	22.6	22.3	0.706	3078.9985
3.881641		1.000000										
4	1	0	1	1	4	0.219113	0.606146	23.904	1.3	1.9	1.067	94.2902
3.719445		1.000000										
5	1	1	0	1	4	0.219121	0.605687	24.122	5.6	6.4	0.989	428.5686
3.686372		1.000000										
6	1	0	1	3	4	0.220683	0.588540	32.252	223.8	241.9	19.348	31419.9473
2.773241		1.000000										
7	1	1	0	3	4	0.220742	0.588190	32.418	236.9	249.7	13.367	33629.4531
2.759450		1.000000										
8	1	1	1	0	4	0.220747	0.588161	32.432	230.0	241.4	11.946	32673.5508
2.758305		1.000000										
9	1	1	1	1	8	0.221085	0.586255	33.336	0.2	0.3	0.037	18.3997

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ZNd123											
2.685555		1.000000									
10	1	1 1	2	8	0.222240	0.580791	35.926	3.7	4.3	1.006	323.6938
2.497610		1.000000									
11	1	0 0	5	2	0.223482	0.576001	38.198	13.9	15.3	1.561	5646.3979
2.354161		1.000000									
12	1	0 1	4	4	0.223490	0.575976	38.210	24.0	26.5	2.794	4872.4272
2.353450		1.000000									
13	1	1 0	4	4	0.223575	0.575674	38.353	18.3	18.7	0.621	3747.8257
2.345004		1.000000									
14	1	1 1	3	8	0.224571	0.572370	39.920	85.0	80.8	4.399	9482.4727
2.256503		1.000000									
15	1	0 1	5	4	0.228435	0.561922	44.873	1.4	1.5	0.266	398.2157
2.018228		1.000000									
16	1	1 0	5	4	0.228547	0.561658	44.999	0.1	0.1	0.021	15.0929
2.012894		1.000000									
17	1	1 1	4	8	0.228557	0.561636	45.009	6.7	8.9	2.946	971.2916
2.012449		1.000000									
18	1	0 0	6	2	0.229697	0.559045	46.238	45.2	48.1	3.088	27903.4219
1.961801		1.000000									
19	1	0 2	0	2	0.229736	0.558958	46.279	72.4	78.7	6.833	44817.1875
1.960155		1.000000									
20	1	2 0	0	2	0.230210	0.557928	46.767	70.0	57.0	10.503	44310.4609
1.940821		1.000000									
21	1	0 2	1	4	0.230395	0.557534	46.954	0.9	1.0	0.099	289.4474
1.933529		1.000000									
22	1	2 0	1	4	0.230879	0.556516	47.437	0.9	0.7	0.180	286.3216
1.914964		1.000000									
23	1	0 2	2	4	0.232455	0.553352	48.937	0.2	0.2	0.174	58.7128
1.859723		1.000000									
24	1	2 0	2	4	0.232969	0.552365	49.405	0.2	1.2	8.088	58.7336
1.843186		1.000000									
25	1	1 1	5	8	0.234751	0.549093	50.956	6.7	7.2	1.057	1277.7816
1.790648		1.000000									
26	1	0 1	6	4	0.236127	0.546707	52.088	4.2	4.6	0.498	1677.4753
1.754393		1.000000									
27	1	0 2	3	4	0.236163	0.546648	52.116	6.1	6.7	0.804	2452.5432
1.753510		1.000000									
28	1	1 0	6	4	0.236267	0.546471	52.200	4.8	5.5	0.819	1950.7393
1.750886		1.000000									
29	1	1 2	0	4	0.236314	0.546392	52.237	6.3	7.4	1.230	2571.0740
1.749716		1.000000									
30	1	2 0	3	4	0.236726	0.545704	52.563	6.0	5.6	0.432	2445.8196
1.739628		1.000000									

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31	1	2	1	0	4	0.236738	0.545684	52.573	8.1	7.6	0.598	3323.5278
1.739341		1.000000										
32	1	1	2	1	8	0.237099	0.545088	52.855	0.7	0.7	0.116	153.0526
1.730700		1.000000										
33	1	2	1	1	8	0.237529	0.544386	53.188	0.2	0.1	0.126	43.9931
1.720657		1.000000										
34	1	0	0	7	2	0.239319	0.541564	54.526	7.7	10.4	3.743	6831.9165
1.681543		1.000000										
35	1	1	2	2	8	0.239531	0.541239	54.681	2.2	2.4	0.370	486.8625
1.677167		1.000000										
36	1	2	1	2	8	0.239983	0.540553	55.006	0.5	0.3	0.207	114.5116
1.668022		1.000000										
37	1	0	2	4	4	0.241911	0.537717	56.350	0.2	0.1	0.106	111.4518
1.631369		1.000000										
38	1	2	0	4	4	0.242541	0.536822	56.775	0.2	0.2	0.070	111.7527
1.620172		1.000000										
39	1	1	1	6	8	0.243806	0.535063	57.609	67.4	69.7	2.503	16976.1797
1.598687		1.000000										
40	1	1	2	3	8	0.243846	0.535008	57.635	84.4	87.6	3.470	21281.4121
1.598019		1.000000										
41	1	2	1	3	8	0.244333	0.534345	57.949	78.7	76.2	2.587	20092.0859
1.590103		1.000000										
42	1	0	1	7	4	0.247305	0.530455	59.794	3.5	4.9	1.944	1936.0344
1.545381		1.000000										
43	1	1	0	7	4	0.247476	0.530239	59.896	5.6	7.5	2.455	3086.4346
1.542982		1.000000										
44	1	0	2	5	4	0.250243	0.526839	61.508	5.5	4.7	0.830	3218.6506
1.506351		1.000000										
45	1	1	2	4	8	0.250436	0.526609	61.617	8.0	8.1	0.468	2338.6228
1.503944		1.000000										
46	1	2	0	5	4	0.250957	0.525990	61.911	5.4	4.9	0.541	3190.4460
1.497522		1.000000										
47	1	2	1	4	8	0.250972	0.525973	61.919	9.7	8.7	0.992	2854.9055
1.497339		1.000000										
48	1	0	0	8	2	0.253195	0.523404	63.137	0.1	0.3	0.824	108.5988
1.471351		1.000000										
49	1	1	1	7	8	0.256552	0.519707	64.890	11.5	11.5	1.101	3750.7466
1.435776		1.000000										
50	1	1	2	5	8	0.259866	0.516249	66.530	0.1	0.1	0.067	34.4629
1.404314		1.000000										
51	1	2	1	5	8	0.260469	0.515639	66.819	0.9	0.3	0.331	304.7231
1.398933		1.000000										
52	1	0	2	6	4	0.261890	0.514220	67.492	25.0	27.2	2.614	17664.6230

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1.386621		1.000000										
53	1	2 0	6	4	0.262713	0.513413	67.875	24.5	25.7	1.291	17527.7363	
1.379725		1.000000										
54	1	2 2	0	4	0.262783	0.513345	67.907	38.8	41.2	2.697	27757.1914	
1.379153		1.000000										
55	1	0 1	8	4	0.262980	0.513153	67.998	3.8	4.1	0.327	2748.2280	
1.377526		1.000000										
56	1	1 0	8	4	0.263188	0.512951	68.093	5.4	5.6	0.262	3905.1638	
1.375826		1.000000										
57	1	2 2	1	8	0.263935	0.512230	68.435	0.5	0.4	0.100	176.5760	
1.369782		1.000000										
58	1	2 2	2	8	0.267481	0.508909	70.010	0.2	0.3	0.398	63.9710	
1.342778		1.000000										
59	1	0 0	9	2	0.272613	0.504361	72.166	0.9	1.2	0.558	1388.8450	
1.307867		1.000000										
60	1	0 3	0	2	0.272786	0.504213	72.236	1.8	2.2	0.592	2842.1367	
1.306770		1.000000										

No. d-hkl	Code	H	K	L	Mult	Hw	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2
		CORR										
61	1	1 2	6	8	0.272938	0.504083	72.298	4.2	5.0	0.966	1710.1821	
1.305805		1.000000										
62	1	2 1	6	8	0.273628	0.503495	72.577	3.8	4.7	1.175	1528.5541	
1.301475		1.000000										
63	1	2 2	3	8	0.273686	0.503446	72.600	5.4	6.7	1.672	2199.7720	
1.301114		1.000000										
64	1	0 3	1	4	0.274061	0.503128	72.751	0.0	0.0	0.005	25.5904	
1.298791		1.000000										
65	1	1 1	8	8	0.274157	0.503047	72.789	1.2	1.2	0.121	474.1385	
1.298201		1.000000										
66	1	3 0	0	2	0.274866	0.502452	73.072	1.4	0.3	0.391	2337.0769	
1.293880		1.000000										
67	1	3 0	1	4	0.276168	0.501372	73.584	0.1	0.0	0.080	74.9966	
1.286134		1.000000										
68	1	0 2	7	4	0.277883	0.499971	74.248	5.6	7.8	3.055	4774.6875	
1.276269		1.000000										
69	1	0 3	2	4	0.277983	0.499890	74.286	0.1	0.2	0.086	111.2729	
1.275703		1.000000										
70	1	2 0	7	4	0.278847	0.499196	74.616	5.5	5.7	0.576	4744.6714	
1.270886		1.000000										
71	1	3 0	2	4	0.280167	0.498147	75.113	0.4	0.3	0.203	341.7683	
1.263702		1.000000										

								ZNd123				
72	1	2	2	4	8	0.283030	0.495922	76.168	0.3	0.0	0.111	118.0547
1.248805		1.000000										
73	1	0	1	9	4	0.284674	0.494675	76.759	7.7	9.3	1.982	6904.8657
1.240648		1.000000										
74	1	0	3	3	4	0.284844	0.494546	76.820	16.0	18.2	2.585	14392.8301
1.239815		1.000000										
75	1	1	0	9	4	0.284929	0.494483	76.850	6.7	7.4	0.792	6024.6670
1.239406		1.000000										
76	1	1	3	0	4	0.285121	0.494338	76.919	16.9	17.5	0.755	15274.7412
1.238472		1.000000										
77	1	1	3	1	8	0.286548	0.493277	77.422	0.1	0.1	0.003	23.6504
1.231673		1.000000										
78	1	3	0	3	4	0.287165	0.492822	77.638	16.2	13.4	2.310	14833.1924
1.228791		1.000000										
79	1	3	1	0	4	0.287187	0.492806	77.645	16.4	13.6	2.353	15090.1279
1.228689		1.000000										
80	1	3	1	1	8	0.288638	0.491748	78.147	0.1	0.1	0.017	23.5279
1.222050		1.000000										
81	1	1	2	7	8	0.290819	0.490184	78.888	4.7	4.3	0.678	2195.6494
1.212415		1.000000										
82	1	1	3	2	8	0.290931	0.490105	78.926	0.3	0.3	0.046	160.2400
1.211930		1.000000										
83	1	2	1	7	8	0.291627	0.489613	79.159	3.1	3.3	0.438	1475.4047
1.208947		1.000000										
84	1	3	1	2	8	0.293099	0.488583	79.647	0.3	0.1	0.192	159.3415
1.202758		1.000000										
85	1	0	3	4	4	0.295176	0.487154	80.325	2.0	2.4	0.715	1973.4962
1.194307		1.000000										
86	1	2	2	5	8	0.296270	0.486412	80.677	4.5	3.9	0.760	2191.1499
1.189985		1.000000										
87	1	3	0	4	4	0.297703	0.485450	81.133	1.7	1.7	0.229	1622.4174
1.184443		1.000000										
88	1	1	1	9	8	0.298412	0.484979	81.357	2.5	2.6	0.186	1255.0134
1.181753		1.000000										
89	1	1	3	3	8	0.298603	0.484852	81.417	9.1	8.6	0.724	4467.0654
1.181034		1.000000										
90	1	0	0	10	2	0.299665	0.484153	81.748	1.3	1.3	0.150	2550.9854
1.177081		1.000000										
91	1	0	2	8	4	0.299762	0.484090	81.778	0.0	0.0	0.004	34.8907
1.176725		1.000000										
92	1	3	1	3	8	0.300908	0.483342	82.133	8.9	8.4	0.902	4428.0000
1.172541		1.000000										
93	1	2	0	8	4	0.300919	0.483335	82.136	0.0	0.0	0.003	34.3187

ZNd123											
1.172502		1.000000									
94	1	0 3	5	4	0.309835	0.477758	84.781	0.3	0.0	0.170	278.4945
1.142549		1.000000									
95	1	1 3	4	8	0.310173	0.477555	84.877	0.9	0.0	0.434	462.9571
1.141497		1.000000									
96	1	3 0	5	4	0.312662	0.476070	85.581	0.1	0.1	0.018	60.1897
1.133903		1.000000									
97	1	3 1	4	8	0.312689	0.476055	85.588	0.9	0.9	0.266	458.1687
1.133824		1.000000									
98	1	2 2	6	8	0.314578	0.474947	86.113	23.4	32.4	12.352	12395.0742
1.128252		1.000000									
99	1	0 1	10	4	0.314885	0.474769	86.198	8.1	11.0	3.855	8605.6016
1.127360		1.000000									
100	1	1 0	10	4	0.315208	0.474582	86.287	5.8	7.4	1.969	6197.3306
1.126428		1.000000									
101	1	1 2	8	8	0.315316	0.474519	86.316	5.3	6.5	1.499	2804.5688
1.126117		1.000000									
102	1	2 1	8	8	0.316290	0.473957	86.583	3.8	3.0	0.662	2039.1823
1.123336		1.000000									
103	1	1 3	5	8	0.326640	0.468226	89.300	1.5	2.1	1.212	801.5325
1.096054		1.000000									
104	1	3 1	5	8	0.329467	0.466731	90.009	1.4	1.0	0.480	794.4810
1.089255		1.000000									
105	1	0 2	9	4	0.330031	0.466437	90.149	1.1	1.1	0.202	1173.8442
1.087930		1.000000									
106	1	0 3	6	4	0.330181	0.466358	90.186	1.3	1.4	0.268	1412.9204
1.087579		1.000000									
107	1	2 0	9	4	0.331470	0.465689	90.503	1.1	1.3	0.324	1170.3464
1.084590		1.000000									
108	1	2 3	0	4	0.331743	0.465548	90.570	2.3	2.7	0.577	2521.4873
1.083965		1.000000									
109	1	1 1	10	8	0.332331	0.465246	90.713	4.4	4.9	0.707	2439.1428
1.082624		1.000000									
110	1	3 0	6	4	0.333443	0.464677	90.983	1.4	1.2	0.200	1539.7311
1.080115		1.000000									
111	1	3 2	0	4	0.333566	0.464614	91.013	1.9	1.6	0.331	2152.1294
1.079840		1.000000									
112	1	2 3	1	8	0.333764	0.464513	91.061	0.0	0.0	0.007	16.8706
1.079397		1.000000									
113	1	3 2	1	8	0.335611	0.463579	91.504	0.1	0.1	0.048	45.0482
1.075324		1.000000									
114	1	0 0	11	2	0.338058	0.462358	92.082	1.6	0.7	0.639	3482.8240
1.070073		1.000000									

115	1	2	2	7	8	0.339832	0.461485	ZNd123 92.496	6.3	8.4	2.802	3560.8481
1.066365		1.000000										
116	1	2	3	2	8	0.339992	0.461407	92.533	0.2	0.2	0.073	100.0479
1.066035		1.000000										
117	1	3	2	2	8	0.341916	0.460472	92.977	0.5	0.5	0.153	264.1322
1.062110		1.000000										
118	1	1	2	9	8	0.349465	0.456909	94.666	7.9	8.1	0.453	4497.9634
1.047563		1.000000										
119	1	1	3	6	8	0.349636	0.456830	94.704	15.5	16.2	0.963	8797.3975
1.047249		1.000000										
120	1	2	1	9	8	0.350689	0.456346	94.933	8.9	9.3	0.469	5067.7246
1.045323		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	0.350964	0.456221	94.993	18.9	19.4	0.721	10739.3652
1.044825		1.000000										
122	1	3	1	6	8	0.352924	0.455330	95.415	15.3	14.9	0.539	8700.6426
1.041314		1.000000										
123	1	3	2	3	8	0.353028	0.455283	95.437	19.5	19.0	0.703	11106.2393
1.041130		1.000000										
124	1	0	1	11	4	0.358161	0.453000	96.520	0.0	0.0	0.017	21.1079
1.032308		1.000000										
125	1	0	3	7	4	0.358448	0.452874	96.580	1.0	1.6	0.987	1199.1967
1.031828		1.000000										
126	1	1	0	11	4	0.358590	0.452812	96.609	0.0	0.0	0.014	17.0743
1.031592		1.000000										
127	1	3	0	7	4	0.362363	0.451180	97.383	1.5	1.2	0.649	1686.5244
1.025447		1.000000										
128	1	2	3	4	8	0.367710	0.448925	98.452	2.5	2.0	0.865	1447.9951
1.017152		1.000000										
129	1	3	2	4	8	0.369999	0.447980	98.900	2.1	2.9	1.190	1215.1216
1.013741		1.000000										
130	1	0	2	10	4	0.373193	0.446681	99.516	1.8	1.3	0.642	2117.9219
1.009114		1.000000										
131	1	2	0	10	4	0.375082	0.445922	99.876	1.8	1.6	0.518	2110.3528
1.006447		1.000000										
132	1	2	2	8	8	0.375242	0.445859	99.906	0.0	0.0	0.012	24.1247
1.006225		1.000000										
133	1	1	1	11	8	0.381594	0.443367	101.087	2.4	2.4	0.428	1378.3110
0.997631		1.000000										
134	1	1	3	7	8	0.381925	0.443239	101.148	4.0	4.0	0.598	2278.0886

ZNd123											
0.997198		1.000000									
135	1	3 1	7	8	0.385925	0.441714	101.871	4.0	4.0	0.719	2257.4131
0.992070		1.000000									
136	1	2 3	5	8	0.392035	0.439443	102.948	0.5	0.0	0.312	260.3880
0.984605		1.000000									
137	1	3 2	5	8	0.394674	0.438484	103.403	0.1	0.0	0.032	76.9123
0.981510		1.000000									
138	1	0 0	12	2	0.395201	0.438294	103.493	0.8	0.4	0.240	1826.9021
0.980900		1.000000									
139	1	0 4	0	2	0.395917	0.438036	103.615	6.5	5.7	1.018	14705.0498
0.980078		1.000000									
140	1	0 3	8	4	0.398589	0.437083	104.067	1.4	2.0	0.907	1584.4993
0.977054		1.000000									
141	1	0 4	1	4	0.398908	0.436970	104.120	0.1	0.1	0.044	86.0392
0.976698		1.000000									
142	1	1 2	10	8	0.398951	0.436955	104.128	8.6	12.1	4.929	4852.7378
0.976650		1.000000									
143	1	2 1	10	8	0.400592	0.436377	104.402	11.6	13.4	2.113	6553.2852
0.974835		1.000000									
144	1	3 0	8	4	0.403547	0.435346	104.890	1.9	1.1	0.474	2104.6772
0.971631		1.000000									
145	1	4 0	0	2	0.404694	0.434951	105.078	6.4	3.3	1.688	14394.9961
0.970410		1.000000									
146	1	4 0	1	4	0.407835	0.433877	105.587	0.1	0.1	0.026	83.9277
0.967129		1.000000									
147	1	0 4	2	4	0.408189	0.433757	105.644	0.1	0.1	0.027	69.4753
0.966765		1.000000									
148	1	4 0	2	4	0.417594	0.430642	107.121	0.1	0.5	2.843	69.4545
0.957482		1.000000									
149	1	0 1	12	4	0.423999	0.428595	108.092	0.2	0.2	0.068	189.8951
0.951566		1.000000									
150	1	1 0	12	4	0.424624	0.428398	108.185	0.2	0.2	0.059	230.6488
0.951005		1.000000									
151	1	0 4	3	4	0.424784	0.428348	108.209	1.7	1.8	0.427	1828.7168
0.950862		1.000000									
152	1	1 4	0	4	0.425465	0.428135	108.310	1.8	1.9	0.331	1966.5139
0.950256		1.000000									
153	1	2 2	9	8	0.426882	0.427692	108.519	1.9	2.0	0.263	1017.4615
0.949002		1.000000									
154	1	2 3	6	8	0.427148	0.427610	108.559	2.3	2.5	0.326	1286.5410
0.948769		1.000000									
155	1	1 3	8	8	0.428605	0.427159	108.773	0.7	0.7	0.102	381.8355
0.947499		1.000000									

								ZNd123				
156	1	1	4	1	8	0.428980	0.427043	108.827	0.1	0.1	0.008	30.5101
0.947174		1.000000										
157	1	3	2	6	8	0.430347	0.426623	109.026	2.5	2.4	0.392	1388.2654
0.946000		1.000000										
158	1	3	1	8	8	0.433790	0.425577	109.523	0.7	0.5	0.179	380.7544
0.943097		1.000000										
159	1	4	0	3	4	0.435083	0.425187	109.707	1.7	1.5	0.312	1813.6587
0.942026		1.000000										
160	1	4	1	0	4	0.435139	0.425171	109.715	2.1	1.9	0.375	2235.9521
0.941980		1.000000										
161	1	0	2	11	4	0.438523	0.424163	110.193	2.4	3.0	0.758	2621.1443
0.939232		1.000000										
162	1	4	1	1	8	0.438839	0.424069	110.237	0.0	0.0	0.006	12.0453
0.938978		1.000000										
163	1	1	4	2	8	0.439934	0.423747	110.390	0.4	0.4	0.081	214.3722
0.938106		1.000000										
164	1	2	0	11	4	0.441234	0.423366	110.571	2.4	2.5	0.470	2607.4412
0.937080		1.000000										
165	1	4	1	2	8	0.450381	0.420743	111.815	0.2	0.0	0.150	86.4077
0.930142		1.000000										
166	1	0	4	4	4	0.450764	0.420635	111.866	0.1	0.0	0.086	103.5419
0.929861		1.000000										
167	1	0	3	9	4	0.458430	0.418515	112.871	3.7	5.6	2.754	3904.4080
0.924414		1.000000										
168	1	1	1	12	8	0.458739	0.418431	112.911	3.8	5.5	2.365	2018.0516
0.924201		1.000000										
169	1	1	4	3	8	0.459678	0.418177	113.031	16.6	20.2	4.482	8689.9746
0.923556		1.000000										
170	1	4	0	4	4	0.462574	0.417397	113.401	0.1	0.1	0.009	102.6000
0.921593		1.000000										
171	1	3	0	9	4	0.465248	0.416685	113.739	3.3	3.0	0.340	3429.3428
0.919817		1.000000										
172	1	3	3	0	4	0.465830	0.416531	113.812	8.5	7.6	0.981	8850.5908
0.919435		1.000000										
173	1	3	3	1	8	0.470156	0.415397	114.349	0.0	0.0	0.005	15.9611
0.916643		1.000000										
174	1	4	1	3	8	0.471245	0.415115	114.483	15.9	13.6	2.157	8210.9336
0.915953		1.000000										
175	1	1	2	11	8	0.476187	0.413848	115.084	0.0	0.1	0.007	25.5885
0.912888		1.000000										
176	1	2	1	11	8	0.478640	0.413229	115.378	0.1	0.1	0.017	32.6826
0.911404		1.000000										
177	1	2	3	7	8	0.479192	0.413090	115.443	1.9	1.4	0.567	990.5110

ZNd123												
No. d-hkl	Code	H	K	L	Mult	HW	ETA/M	2theta/TOF	Icalc	Iobs	Sigma	StrFactor^2
0.911074	1	1.000000										
178		3	2	7	8	0.483357	0.412054	115.935	2.7	2.3	0.640	1366.8093
0.908621	1	1.000000										
179		3	3	2	8	0.483710	0.411967	115.976	0.3	0.2	0.056	128.9278
0.908417	1	1.000000										
180		0	0	13	2	0.488926	0.410693	116.580	2.4	2.6	0.443	4881.7725
0.905447	1	1.000000										
181	1	0	4	5	4	0.490086	0.410413	116.713	1.3	1.2	0.199	1280.9440
0.904799	1	1.000000										
182		1	4	4	8	0.491030	0.410186	116.820	1.9	1.6	0.380	953.5997
0.904277	1	1.000000										
183		1	3	9	8	0.500392	0.407979	117.867	1.9	1.1	0.707	946.4503
0.899264	1	1.000000										
184		4	0	5	4	0.504464	0.407043	118.311	1.3	1.3	0.174	1258.0725
0.897176	1	1.000000										
185		4	1	4	8	0.504542	0.407025	118.319	2.2	2.3	0.305	1102.3073
0.897137	1	1.000000										
186		3	1	9	8	0.507815	0.406283	118.671	1.9	2.3	0.444	941.5601
0.895498	1	1.000000										
187		2	2	10	8	0.508167	0.406203	118.709	3.6	4.2	0.715	1772.7410
0.895324	1	1.000000										
188		3	3	3	8	0.508448	0.406140	118.739	6.3	7.1	1.058	3113.1240
0.895185	1	1.000000										

 BRAGG R-Factors and weight fractions for Pattern # 1

=> Phase: 1 ZNd123
 => Bragg R-factor: 8.29 Vol: 179.119(0.000) Fract(%): 100.00(0.00)
 => Rf-factor= 8.53 ATZ: 718.629 Brindley: 1.0000

 CPU Time: 2.844 seconds
 0.047 minutes

=> Run finished at: Date: 12/12/2017 Time: 09:46:06.729^{ZNd123}