

CELL PROPOSALS FROM THE ORGANIZERS

(Samples 1 to 8)

SAMPLE-1

No zeropoint detected.

No result in cubic, tetragonal, hexagonal, and orthorhombic tests..

TREOR

Data :

Sample 1

11.950
13.299
13.610
17.164
17.915
18.149
20.809
23.260
23.629
24.042
25.431
25.722
26.782
27.582
27.722
28.169
29.430
29.697
30.694
34.696

CHOICE=3, WAVE=1.54056,
CEM=20.0, VOL=-1000, D2=0.0004, D1=0.0002,
END*
-.000

Result :

Solution in P2/n :

TOTAL NUMBER OF LINES = 20

A = 10.323388 .002587 A ALFA = 90.000000 .000000 DEG
B = 7.395172 .002097 A BETA = 91.295975 .020152 DEG
C = 8.535501 .002450 A GAMMA = 90.000000 .000000 DEG

UNIT CELL VOLUME = 651.46 A**3

H	K	L	SST-OBS	SST-CALC	DELTA	2TH-OBS	2TH-CALC	D-OBS	FREE PARAM.
0	1	0	.010844	.010849	-.000005	11.955	11.958	7.3969	
-1	0	1	.013409	.013414	-.000005	13.299	13.302	6.6520	
1	0	1	.014040	.014023	.000017	13.610	13.602	6.5008	
2	0	0	.022227	.022281	-.000054	17.148	17.169	5.1666	
-1	1	1	.024243	.024263	-.000020	17.915	17.922	4.9471	
1	1	1	.024875	.024872	.000003	18.149	18.148	4.8839	
0	0	2	.032615	.032593	.000022	20.809	20.802	4.2652	
-2	1	1	.040639	.040669	-.000030	23.260	23.269	3.8210	
2	1	1	.041920	.041888	.000032	23.629	23.620	3.7622	
0	2	0	.043376	.043397	-.000021	24.042	24.048	3.6985	

0	1	2		.043442				24.060	
-1	1	2	.048448	.048403	.000046	25.431	25.419	3.4995	
1	1	2	.049545	.049622	-.000077	25.722	25.742	3.4606	
-2	0	2	.053636	.053655	-.000019	26.782	26.787	3.3260	
-1	2	1	.056825	.056811	.000015	27.582	27.578	3.2313	
-3	0	1	.057392	.057366	.000026	27.722	27.716	3.2153	
1	2	1		.057420				27.729	
3	0	1	.059221	.059195	.000026	28.169	28.163	3.1653	
-2	1	2	.064522	.064504	.000018	29.430	29.426	3.0325	
2	2	0	.065671	.065678	-.000007	29.697	29.699	3.0058	
3	1	1	.070047	.070044	.000003	30.694	30.693	2.9104	
-1	1	3	.088908	.088839	.000069	34.696	34.682	2.5833	
4	0	0		.089124				34.739	

NUMBER OF OBS. LINES = 20
 NUMBER OF CALC. LINES = 23
 M(20)= 35 AV.EPS.= .0000256
 F 20 = 56.(.007377, 49)
 M(20)= 35 AV.EPS.= .0000256
 F 20 = 56.(.007377, 49)
 M CF. J.APPL.CRYST. 1(1968)108
 F CF. J.APPL.CRYST. 12(1979)60
 0 LINES ARE UNINDEXED

DICVOL

Data :

Sample 1
 20 2 0 0 0 0 1 0
 20. 15. 15. 0. 1000. 90. 130.
 1.54056 0. 0. 0.
 0.03 0. 0.0
 11.950
 13.299
 13.610
 17.164
 17.915
 18.149
 20.809
 23.260
 23.629
 24.042
 25.431
 25.722
 26.782
 27.582
 27.722
 28.169
 29.430
 29.697
 30.694
 34.696

Results :

Solution in P2/n :

M O N O C L I N I C S Y S T E M

DIRECT PARAMETERS : A=10.3238 B= 7.3961 C= 8.5335 BETA= 91.302 VOLUME= 651.41

STANDARD DEVIATIONS : 0.0024 0.0021 0.0018 0.019

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
0	1	0	7.39981	7.39613	0.00368	0.018260	.01828	11.950	11.956	-0.006
1	0	-1	6.65208	6.65031	0.00177	0.022600	.02261	13.299	13.303	-0.004
1	0	1	6.50077	6.50351	-0.00275	0.023660	.02364	13.610	13.604	0.006
2	0	0	5.16188	5.16054	0.00134	0.037530	.03755	17.164	17.168	-0.004
1	1	-1	4.94715	4.94520	0.00195	0.040860	.04089	17.915	17.922	-0.007
1	1	1	4.88389	4.88394	-0.00005	0.041920	.04192	18.149	18.149	0.000
0	0	2	4.26520	4.26565	-0.00045	0.054970	.05496	20.809	20.807	0.002
2	1	-1	3.82101	3.81975	0.00126	0.068490	.06854	23.260	23.268	-0.008
2	1	1	3.76217	3.76349	-0.00132	0.070650	.07060	23.629	23.621	0.008
0	1	2	3.69847	3.69514	0.00333	0.073110	.07324	24.042	24.064	-0.022
0	2	0		3.69807	0.00040		0.07312		24.045	-0.003
1	1	-2	3.49952	3.50084	-0.00131	0.081650	.08159	25.431	25.421	0.010
1	1	2	3.46059	3.45737	0.00322	0.083500	.08366	25.722	25.746	-0.024
2	0	-2	3.32598	3.32515	0.00082	0.090400	.09044	26.782	26.789	-0.007
1	2	-1	3.23130	3.23198	-0.00068	0.095770	.09573	27.582	27.576	0.006
1	2	1	3.21530	3.21470	0.00060	0.096730	.09677	27.722	27.727	-0.005
3	0	-1		3.21614	-0.00084		0.09668		27.715	0.007
3	0	1	3.16528	3.16584	-0.00055	0.099810	.09978	28.169	28.164	0.005
2	1	-2	3.03246	3.03276	-0.00029	0.108740	.10872	29.430	29.427	0.003
2	2	0	3.00581	3.00594	-0.00014	0.110680	.11067	29.697	29.696	0.001
3	1	1	2.91041	2.91042	-0.00002	0.118060	.11806	30.694	30.694	0.000
1	1	-3	2.58332	2.58393	-0.00061	0.149850	.14977	34.696	34.688	0.008

* NUMBER OF LINES

.- INPUT DATA = 20
.- CALCULATED = 49

* MEAN ABSOLUTE DISCREPANCIES

<Q> =0.3505E-04
<DELTA(2-THETA)> =0.5905E-02
MAX. ERROR ACCEPTED (DEG. 2-THETA) =0.4500E-01

* FIGURES OF MERIT

1.- M(20) = 43.6 (REF. 4)
2.- F(20) = 69.1(0.0059, 49) (REF. 5)

Solution in P2/a :

M O N O C L I N I C S Y S T E M

DIRECT PARAMETERS : A=13.2437 B= 7.3961 C= 8.5335 BETA=128.802 VOLUME= 651.41
STANDARD DEVIATIONS : 0.0027 0.0021 0.0018 0.019

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
0	1	0	7.39981	7.39613	0.00368	0.018260	.01828	11.950	11.956	-0.006
0	0	1	6.65208	6.65031	0.00177	0.022600	.02261	13.299	13.303	-0.004
2	0	-1	6.50077	6.50351	-0.00275	0.023660	.02364	13.610	13.604	0.006
2	0	0	5.16188	5.16054	0.00134	0.037530	.03755	17.164	17.168	-0.004
0	1	1	4.94715	4.94520	0.00195	0.040860	.04089	17.915	17.922	-0.007
2	1	-1	4.88389	4.88394	-0.00005	0.041920	.04192	18.149	18.149	0.000
2	0	-2	4.26520	4.26565	-0.00045	0.054970	.05496	20.809	20.807	0.002
1	1	1	3.82101	3.81975	0.00126	0.068490	.06854	23.260	23.268	-0.008
3	1	-1	3.76217	3.76349	-0.00132	0.070650	.07060	23.629	23.621	0.008

0	2	0	3.69847	3.69807	0.00040	0.073110.07312	24.042	24.045	-0.003
2	1	-2		3.69514	0.00333	0.07324		24.064	-0.022
1	1	-2	3.49952	3.50084	-0.00131	0.081650.08159	25.431	25.421	0.010
3	1	-2	3.46059	3.45737	0.00322	0.083500.08366	25.722	25.746	-0.024
0	0	2	3.32598	3.32515	0.00082	0.090400.09044	26.782	26.789	-0.007
0	2	1	3.23130	3.23198	-0.00068	0.095770.09573	27.582	27.576	0.006
2	0	1	3.21530	3.21614	-0.00084	0.096730.09668	27.722	27.715	0.007
2	2	-1		3.21469	0.00060	0.09677		27.727	-0.005
4	0	-1	3.16528	3.16584	-0.00055	0.099810.09978	28.169	28.164	0.005
0	1	2	3.03246	3.03276	-0.00029	0.108740.10872	29.430	29.427	0.003
2	2	0	3.00581	3.00594	-0.00014	0.110680.11067	29.697	29.696	0.001
4	1	-1	2.91041	2.91042	-0.00002	0.118060.11806	30.694	30.694	0.000
2	1	-3	2.58332	2.58393	-0.00061	0.149850.14977	34.696	34.688	0.008

* NUMBER OF LINES

.- INPUT DATA = 20

.- CALCULATED = 49

* MEAN ABSOLUTE DISCREPANCIES

<Q> =0.3505E-04

<DELTA(2-THETA)> =0.5905E-02

MAX. ERROR ACCEPTED (DEG. 2-THETA) =0.4500E-01

* FIGURES OF MERIT

1.- M(20) = 43.6 (REF. 4)

2.- F(20) = 69.1(0.0059, 49) (REF. 5)

McMAILLE

Data :

SDPDRR-2 sample 1

! Wavelength, zeropoint and NGRID

1.54056 0.0 0

! Symmetry codes

0 0 0 0 1 0

! W, Nind

0.24 4

! Pmin, Pmax, Vmin, Vmax, Rp min, Rp max

5. 15. 100. 800. 0.10 0.50

! N of Monte Carlo events, number of runs

10000000 5

! Couples of 2-theta and intensities

!	2Theta	Height	Area	FWHM
	11.950	850,1	5882,2	0,1400
	13.299	5274,1	31622,3	0,1200
	13.610	3955,3	27061,2	0,1400
	17.164	4982,7	29782,7	0,1200
	17.915	576,4	4026,2	0,1400
	18.149	488,9	3382,3	0,1400
	20.809	3770,5	25935,1	0,1400
	23.260	427,8	3422,4	0,1600
	23.629	710,8	4922,0	0,1400
	24.042	1049,6	8390,8	0,1600
	25.431	748,7	5957,0	0,1600
	25.722	429,5	3273,2	0,1600
	26.782	605,8	4844,4	0,1600
	27.582	3205,5	18418,9	0,1200

27.722	3422,5	19890,5	0,1200
28.169	646,7	5776,4	0,1800
29.430	403,4	3204,3	0,1600
29.697	773,9	5410,3	0,1400
30.694	165,1	986,8	0,1200
34.696	646,5	5810,5	0,1800

Result :

ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
0.008	1.5406	10.3198	7.3943	8.5312	90.000	91.299	90.000
0.007	0.0000	0.0035	0.0028	0.0030	0.000	0.017	0.000
RECIPROCAL CELL :		0.09693	0.13524	0.11725	90.000	88.701	90.000
VOLUME (A**3) :		650.831					

H	K	L	TH(OBS)	TH-ZERO	TH(CALC)	DIFF.
0	1	0	11.950	11.958	11.959	-0.001
1	0	-1	13.299	13.307	13.307	-0.001
1	0	1	13.610	13.618	13.608	0.009
2	0	0	17.164	17.172	17.175	-0.003
1	1	-1	17.915	17.923	17.928	-0.005
1	1	1	18.149	18.157	18.154	0.003
0	0	2	20.809	20.817	20.812	0.004
2	1	-1	23.260	23.268	23.276	-0.008
2	1	1	23.629	23.637	23.628	0.009
0	2	0	24.042	24.050	24.051	-0.001
1	1	-2	25.431	25.439	25.429	0.010
1	1	2	25.722	25.730	25.753	-0.024
2	0	-2	26.782	26.790	26.798	-0.008
1	2	-1	27.582	27.590	27.584	0.006
3	0	-1	27.722	27.730	27.725	0.004
3	0	1	28.169	28.177	28.174	0.003
2	1	-2	29.430	29.438	29.437	0.001
2	2	0	29.697	29.705	29.705	0.000
3	1	1	30.694	30.702	30.704	-0.003
1	1	-3	34.696	34.704	34.698	0.006

M(20) =	47.22789	
F(20) =	75.03664	(5.4395199E-03, 49)

=====

FINAL LIST OF CELL PROPOSALS, sorted by Rp :

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Rp	Vol	Vol/V1	Ind	Nsol	a	b	c	alpha	beta	gamma
0.041	650.914	1.00	20	1	10.3203	7.3942	8.5321	90.000	91.316	90.000
0.123	790.827	1.21	17	1	7.1638	7.4414	14.8376	90.000	91.132	90.000
0.160	783.034	1.20	16	1	14.8058	7.2038	7.3449	90.000	91.724	90.000
0.196	682.996	1.05	18	1	6.9412	7.3966	13.4434	90.000	98.287	90.000

FULLPROF

Cell confirmation and structure factors extraction (Le Bail fit).

Description in the standard space group P2/c
(of course, the structure could be acentric as well in the Pc space group) :

Summary file (reduced) :

=> Phase No. 1 P 2/c

=> No. of reflections for pattern#: 1: 375/2

==> PROFILE PARAMETERS FOR PATTERN# 1

=> Cell parameters :

8.52850	0.00080
7.39479	0.00073
13.23662	0.00126
90.00000	0.00000
128.76793	0.00253
90.00000	0.00000

=> overall scale factor : 0.000010000 0.000000000

=> Eta(p-v) or m(p-vii) : 0.67178 0.01346

=> Halfwidth parameters : 0.01362 0.00000
0.06704 0.00000
0.00404 0.00028

=> Asymmetry parameters : 0.00806 0.00662
0.00333 0.00091

=> Phase No. 2 Pyrochlore F D 3 M

=> No. of reflections for pattern#: 1: 30/2

==> ATOM PARAMETERS:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.	Mult
Al	0.00000(0)		0.00000(0)		0.00000(0)		0.800(0)		0.160(0)		16
F	0.31660(0)		0.12500(0)		0.12500(0)		1.800(0)		0.480(0)		48

==> PROFILE PARAMETERS FOR PATTERN# 1

=> Cell parameters :

9.82108	0.00080
9.82108	0.00080
9.82108	0.00080
90.00000	0.00000
90.00000	0.00000
90.00000	0.00000

=> overall scale factor : 0.000021918 0.000000178

=> Eta(p-v) or m(p-vii) : 0.76843 0.02603

=> Halfwidth parameters : 0.01362 0.00000
0.06704 0.00000
0.00779 0.00063

==> GLOBAL PARAMETERS FOR PATTERN# 1

=> Zero-point: -0.0065 0.0031

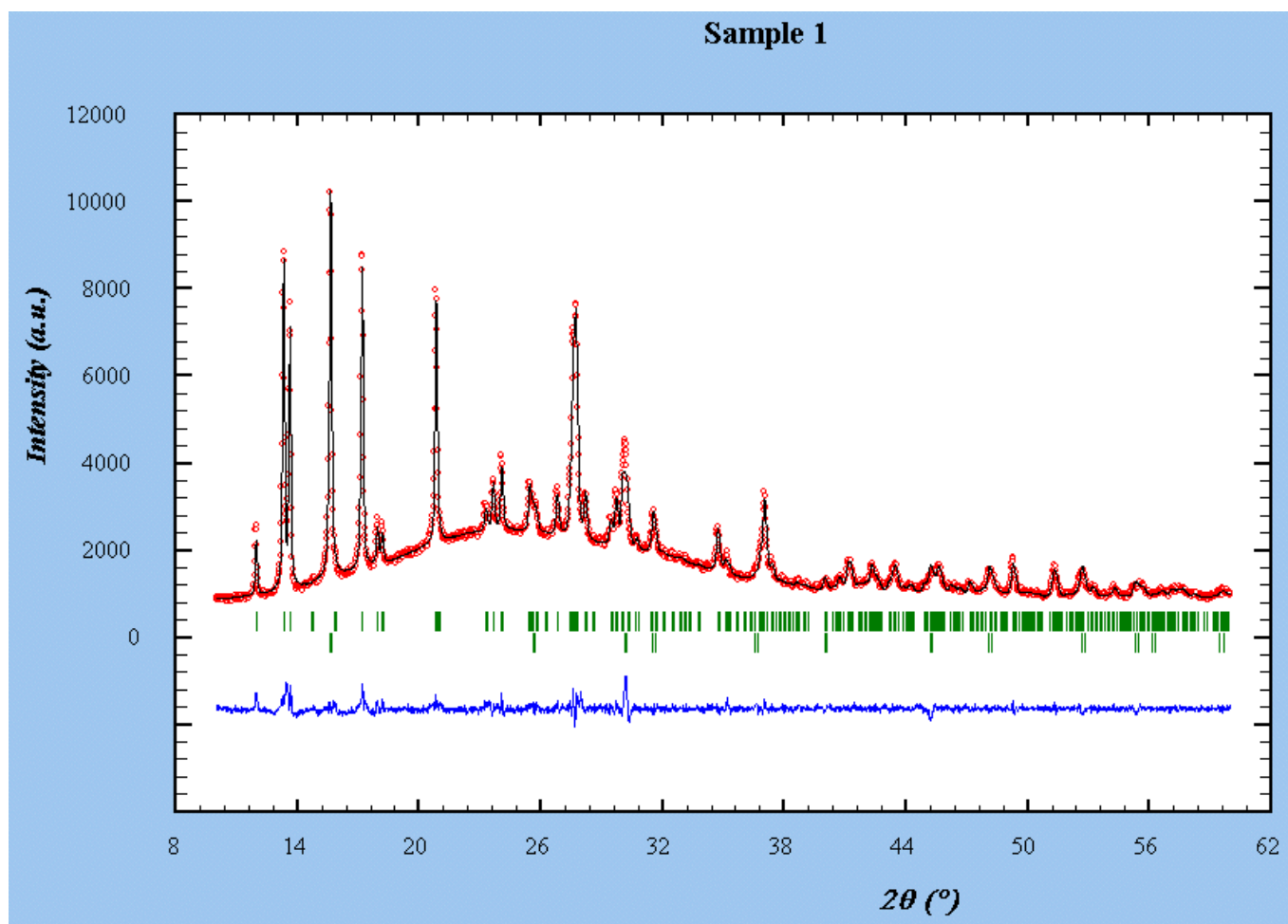
==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS FOR PATTERN: 1

```

=> N-P+C: 2368
=> R-factors (not corrected for background) for Pattern: 1
=> Rp: 2.93      Rwp: 4.12      Rexp: 2.36 Chi2: 3.05      M.L. refinement
=> Conventional Rietveld R-factors for Pattern: 1
=> Rp: 14.5      Rwp: 13.4      Rexp: 7.68 Chi2: 3.05
=> Deviance: 0.711E+04      Dev* : 3.004
=> DW-Stat.: 0.7723      DW-exp: 1.8835
=> N-sigma of the GoF: 70.441

=> Global user-weighted Chi2 (Bragg contrib.):3.11
=> Phase: 1
=> Bragg R-factor: 3.42      Vol: 650.874 ( 0.108)      Fract(%): 0.00 (NaN )
=> Rf-factor= 2.05      ATZ: 744.080      Brindley: 1.0000
=> Phase: 2
=> Bragg R-factor: 5.52      Vol: 947.278 ( 0.134)      Fract(%): 100.00 (NaN )
=> Rf-factor= 3.20      ATZ: 1343.630      Brindley: 1.0000

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SAMPLE-2

No zeropoint detected.

No result in cubic, tetragonal, hexagonal, and orthorhombic tests..

TREOR

Data :

Sample 2
4.246
4.786
5.408
6.070
7.008
7.353
7.773
7.797
8.469
8.497
9.099
9.295
9.581
9.874
10.828
10.895
10.953
10.999
11.094
11.171
11.426

CHOICE=3, WAVE=0.79764,
CEM=20.0, VOL=-2000, D2=0.0002, D1=0.0001,
END*
-.000

Result :

TOTAL NUMBER OF LINES = 21
A = 19.873476 .064836 A ALFA = 90.000000 .000000 DEG
B = 8.195149 .011105 A BETA = 106.019691 .513029 DEG
C = 11.237923 .041775 A GAMMA = 90.000000 .000000 DEG
UNIT CELL VOLUME = 1759.20 A**3
H K L SST-OBS SST-CALC DELTA 2TH-OBS 2TH-CALC D-OBS FREE PARAM.
0 0 1 .001363 .001363 .000000 4.232 4.232 10.8025
-1 0 1 .001374 .001374 4.248
2 0 0 .001744 .001744 .000000 4.786 4.786 9.5511
1 0 1 .002226 .002225 .000001 5.408 5.407 8.4539
-2 0 1 .002256 .002256 5.445
1 1 0 .002803 .002804 -.000001 6.070 6.071 7.5326
0 1 1 .003735 .003732 .000004 7.008 7.004 6.5254
-1 1 1 .003742 .003742 7.014
2 1 0 .004112 .004112 .000000 7.353 7.353 6.2196
1 1 1 .004594 .004593 .000001 7.773 7.772 5.8840
-2 1 1 .004623 .004624 -.000002 7.797 7.799 5.8659
0 0 2 .005452 .005453 -.000001 8.469 8.470 5.4012
-2 0 2 .005488 .005495 -.000007 8.497 8.502 5.3835
3 1 0 .006292 .006292 .000000 9.099 9.099 5.0280
2 1 1 .006326 .006326 9.124
-3 1 1 .006378 .006378 9.162

3	0	1	.006565	.006563	.000002	9.295	9.294	4.9222
-4	0	1		.006636			9.345	
4	0	0	.006974	.006975	.000000	9.581	9.581	4.7756
-1	1	2	.007406	.007406	.000000	9.874	9.874	4.6342
2	0	2	.008902	.008899	.000003	10.828	10.826	4.2270
3	1	1		.008931			10.846	
-4	1	1	.009012	.009004	.000008	10.895	10.890	4.2010
-4	0	2		.009024			10.902	
1	1	2	.009108	.009108	.000000	10.953	10.953	4.1789
-3	1	2	.009185	.009192	-.000007	10.999	11.003	4.1614
4	1	0	.009344	.009343	.000001	11.094	11.094	4.1259
0	2	0	.009473	.009473	.000000	11.171	11.171	4.0976
1	2	0	.009909	.009909	.000000	11.426	11.426	4.0064

NUMBER OF OBS. LINES = 21
 NUMBER OF CALC. LINES = 29
 M(20)= 65 AV.EPS.= .0000019
 F 20 = 374.(.001410, 38)
 M(21)= 69 AV.EPS.= .0000018
 F 21 = 400.(.001346, 39)
 M CF. J.APPL.CRYST. 1(1968)108
 F CF. J.APPL.CRYST. 12(1979)60
 0 LINES ARE UNINDEXED

DICVOL

Data :

Sample 2
 21 2 0 0 0 0 1 0
 25. 25. 25. 0. 2000. 90. 130.
 0.79764 0. 0. 0.
 0.01 0. 0.0
 4.246
 4.786
 5.408
 6.070
 7.008
 7.353
 7.773
 7.797
 8.469
 8.497
 9.099
 9.295
 9.581
 9.874
 10.828
 10.895
 10.953
 10.999
 11.094
 11.171
 11.426

Results :

Could be P21/n space group

M O N O C L I N I C S Y S T E M

DIRECT PARAMETERS : A=19.8782 B= 8.1950 C=11.2411 BETA=106.061 VOLUME=1759.73
 STANDARD DEVIATIONS : 0.0010 0.0003 0.0005 0.004

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
1	0	-1	10.76587	10.76535	0.00051	0.008630	.00863	4.246	4.246	0.000
2	0	0	9.55175	9.55116	0.00059	0.010960	.01096	4.786	4.786	0.000
1	0	1	8.45384	8.45409	-0.00025	0.013990	.01399	5.408	5.408	0.000
1	1	0	7.53258	7.53123	0.00136	0.017620	.01763	6.070	6.071	-0.001
0	1	1	6.52539	6.52887	-0.00348	0.023480	.02346	7.008	7.004	0.004
1	1	-1		6.52067	0.00472		0.02352		7.013	-0.005
2	1	0	6.21961	6.21945	0.00016	0.025850	.02585	7.353	7.353	0.000
1	1	1	5.88402	5.88421	-0.00019	0.028880	.02888	7.773	7.773	0.000
2	1	-1	5.86593	5.86626	-0.00032	0.029060	.02906	7.797	7.797	0.000
0	0	2	5.40123	5.40118	0.00005	0.034280	.03428	8.469	8.469	0.000
2	0	-2	5.38347	5.38268	0.00079	0.034500	.03451	8.497	8.498	-0.001
3	1	0	5.02797	5.02808	-0.00011	0.039560	.03955	9.099	9.099	0.000
3	0	1	4.92217	4.92197	0.00020	0.041270	.04128	9.295	9.295	0.000
4	0	0	4.77557	4.77558	-0.00002	0.043850	.04385	9.581	9.581	0.000
1	1	-2	4.63419	4.63508	-0.00089	0.046560	.04655	9.874	9.872	0.002
2	0	2	4.22696	4.22704	-0.00009	0.055970	.05597	10.828	10.828	0.000
4	1	-1	4.20104	4.20399	-0.00295	0.056660	.05658	10.895	10.887	0.008
4	0	-2		4.20054	0.00050		0.05667		10.896	-0.001
1	1	2	4.17886	4.17858	0.00028	0.057260	.05727	10.953	10.954	-0.001
3	1	-2	4.16144	4.16146	-0.00002	0.057740	.05774	10.999	10.999	0.000
4	1	0	4.12591	4.12611	-0.00020	0.058740	.05874	11.094	11.093	0.001
0	2	0	4.09756	4.09751	0.00005	0.059560	.05956	11.171	11.171	0.000
1	2	0	4.00641	4.00638	0.00003	0.062300	.06230	11.426	11.426	0.000

* NUMBER OF LINES

.- INPUT DATA = 21
 .- CALCULATED = 39

* MEAN ABSOLUTE DISCREPANCIES

<Q> =0.5085E-05
 <DELTA(2-THETA)> =0.6319E-03
 MAX. ERROR ACCEPTED (DEG. 2-THETA) =0.2500E-01

* FIGURES OF MERIT

1.- M(21) = 157.1 (REF. 4)
 2.- F(21) = 852.2(0.0006, 39) (REF. 5)

ITO13

Data :

Sample 2
 9009 1 1 1 0.79764 1.00
 0.000
 4.246
 4.786
 5.408
 6.070
 7.008
 7.353
 7.773
 7.797

8.469
8.497
9.099
9.295
9.581
9.874
10.828
10.895
10.953
10.999
11.094
11.171
11.426
0.0
END

Results :

THE 9 MOST PROBABLE SOLUTIONS

Q(A)	Q(B)	Q(C)	Q(D)	Q(E)	Q(F)	LINES INDEXED	FIGURE OF MERIT	PEDIGREE	BRAVAIS LATTICE	ZEROSHIFT
27.41	148.94	85.71	0.00	26.82	0.00	20.	131.4	252.	P	-0.0010
27.41	148.94	85.71	0.00	26.82	0.00	20.	119.8	251.	P	-0.0009
27.41	148.94	85.71	0.00	26.82	0.00	20.	80.8	226.	P	-0.0009
21.43	37.24	27.41	0.00	13.42	0.00	20.	71.7	337.	C	-0.0017
148.95	27.41	85.72	26.84	55.83	0.00	18.	74.5	561.	P	-0.0005
66.12	63.58	109.53	3.13	58.94	43.60	17.	27.4	253.	P	0.0031
58.67	27.41	141.37	13.28	51.05	13.29	17.	18.7	132.	P	-0.0026
21.59	37.13	27.41	0.00	13.24	0.00	19.	8.4	336.	P	-0.0004
58.68	27.41	141.26	13.30	51.01	13.30	17.	13.3	131.	P	-0.0023

THE DIRECT CONSTANTS OF THESE LATTICES

A	B	C	ALFA	BETA	GAMMA	VOLUME
19.875	8.194	11.240	90.000	106.061	90.000	1759.08
19.875	8.194	11.240	90.000	106.061	90.000	1759.12
19.876	8.194	11.240	90.000	106.062	90.000	1759.18
22.480	16.388	19.875	90.000	106.065	90.000	7035.97
8.479	19.932	11.631	106.603	104.899	85.787	1820.41
14.003	13.398	10.248	83.654	111.164	110.582	1678.22
13.740	19.408	8.780	93.648	105.533	98.177	2219.91
22.364	16.411	19.851	90.000	105.786	90.000	7010.85
13.739	19.408	8.782	93.659	105.523	98.181	2220.64

McMAILLE

Data :

SDPDRR-2 sample 2
! Wavelength, zeropoint and NGRID
0.79764 0.0 0
! Symmetry codes
0 0 0 0 1 0
! W, Nind
0.08 2
! Pmin, Pmax, Vmin, Vmax, Rp min, Rp max
5. 25. 1000. 2000. 0.10 0.50
! N of Monte Carlo events, number of runs
10000000 10
! Couples of 2-theta and intensities

!	2Theta	Height	Area	FWHM
	4.246	4543,7	22631,6	0,0250
	4.786	2660,0	13163,6	0,0250
	5.408	9094,7	43745,7	0,0250
	6.070	590,5	3540,0	0,0300
	7.008	870,1	5202,9	0,0300
	7.353	1751,2	8614,8	0,0250
	7.773	403,2	1993,3	0,0250
	7.797	323,0	1219,8	0,0200
	8.469	2096,2	9632,3	0,0250
	8.497	2534,6	12194,8	0,0250
	9.099	785,0	3878,9	0,0250
	9.295	2298,3	13776,2	0,0300
	9.581	3034,9	18146,5	0,0300
	9.874	328,3	1473,6	0,0250
	10.176	91,4	410,0	0,0250
	10.828	4638,2	22248,7	0,0250
	10.895	5611,4	33622,0	0,0300
	10.953	738,9	3644,1	0,0250
	10.999	992,1	4909,4	0,0250
	11.094	1098,3	5435,0	0,0250
	11.171	2263,3	11210,5	0,0250
	11.426	2092,2	10352,7	0,0250

Results :

ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
0.002	0.7976	11.2385	8.1938	19.9429	90.000	106.727	90.000
0.002	0.0000	0.0022	0.0015	0.0041	0.000	0.009	0.000
RECIPROCAL CELL :		0.09291	0.12204	0.05236	90.000	73.273	90.000
VOLUME (A**3) :		1758.753					

H	K	L	TH(OBS)	TH-ZERO	TH(CALC)	DIFF.
1	0	0	4.246	4.248	4.247	0.001
0	0	2	4.786	4.788	4.787	0.001
1	0	-2	5.408	5.410	5.409	0.001
0	1	1	6.070	6.072	6.072	0.000
1	1	0	7.008	7.010	7.014	-0.005
0	1	2	7.353	7.355	7.354	0.000
1	1	-2	7.773	7.775	7.774	0.001
1	1	1	7.797	7.799	7.798	0.001
2	0	-2	8.469	8.471	8.471	0.000
2	0	0	8.497	8.499	8.500	-0.001
0	1	3	9.099	9.101	9.100	0.000
1	0	-4	9.295	9.297	9.297	0.000
0	0	4	9.581	9.583	9.583	0.000
2	1	-1	9.874	9.876	9.874	0.002
2	1	0	10.176	10.178	10.174	0.004
2	0	-4	10.828	10.830	10.830	0.000
2	0	2	10.895	10.897	10.898	-0.002
2	1	-3	10.953	10.955	10.956	-0.001
2	1	1	10.999	11.001	11.001	0.000
0	1	4	11.094	11.096	11.095	0.000
0	2	0	11.171	11.173	11.173	0.000
0	2	1	11.426	11.428	11.428	0.000

M(20) = 90.56862

F(20) = 509.8503 (1.0601947E-03, 37)

=====

FINAL LIST OF CELL PROPOSALS, sorted by Rp :

```

=====
Rp      Vol      Vol/V1  Ind  Nsol      a          b          c      alpha  beta  gamma
0.029   1760.496  1.00   22    1  11.2403   8.1983   19.9471  90.000 106.714 90.000

```

```

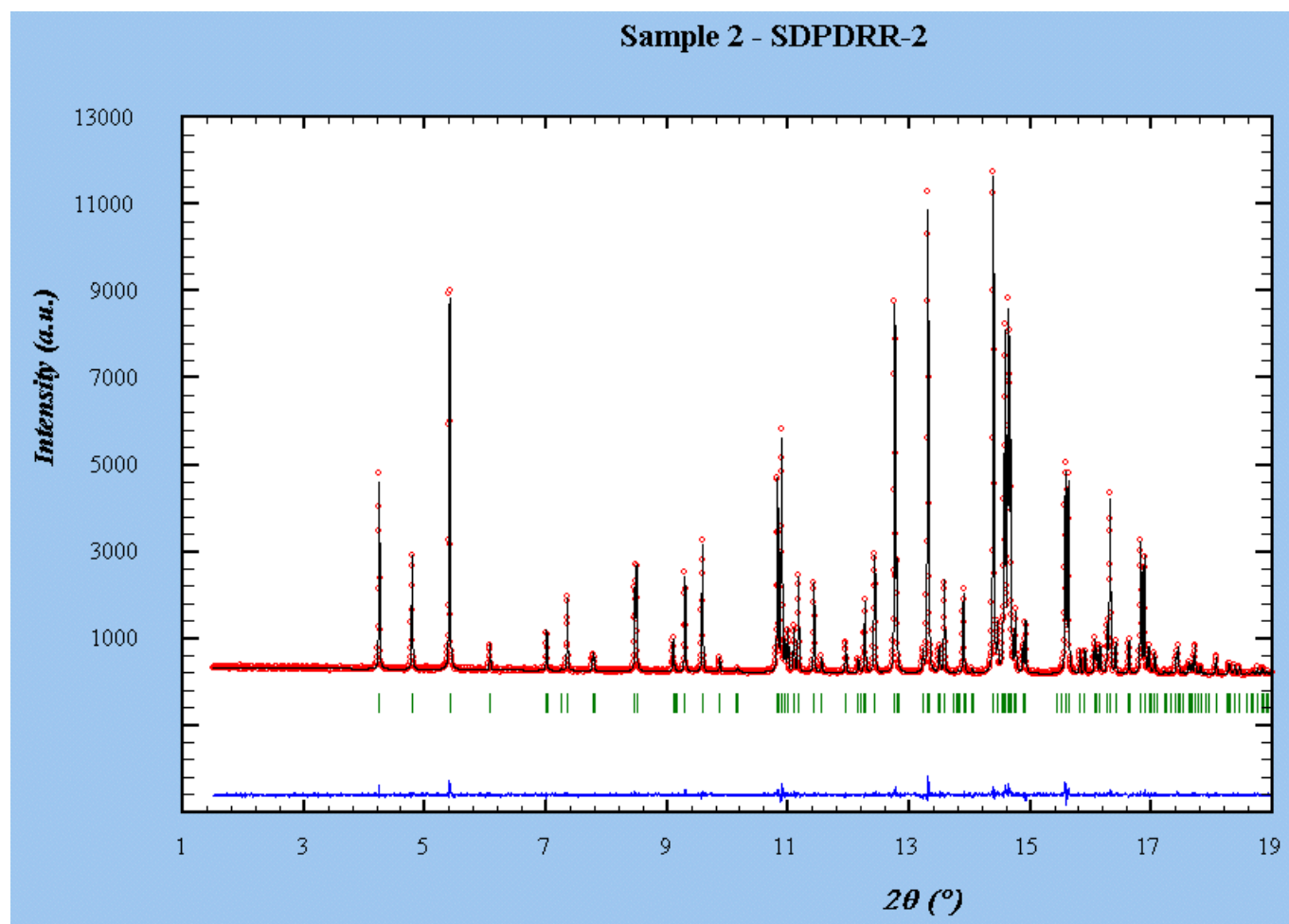
Final Rp on the .prf = 8.4556095E-02

```

FULLPROF

Cell confirmation and structure factors extraction (Le Bail fit).

Description in the standard space group $P2_1/c$



SAMPLE-3

No zeropoint detected.

McMAILLE

Data :

```
Sample 3 SDPDRR-2
! Wavelength, zeropoint and NGRID
0.79764 0.0 2
! Symmetry codes
1 0 0 0 0 0
! W
0.04 2
! Pmin, Pmax Vmin, Vmax, Rp min, Rp max
3. 30. 200. 20000. 0.02 0.50
! Step on a, b, c parameters, step on angles
0.01 0.2
! N of Monte Carlo events and Nruns
2000 1
! Couples of 2-theta and intensities
!   2Theta      Height      Area      FWHM
   3.419        1154,8      7998,7      0,0700
   4.839        17132,7    101978,3     0,0600
   5.929        21795,5    129179,6     0,0600
   7.656         429,1      2437,5      0,0600
   8.390         951,0      5698,4      0,0600
   9.061        20957,1    124984,8     0,0600
   9.690        2684,7     16088,6     0,0600
  10.280        21990,8    671176,9     0,0600
  11.369        20816,3    124080,4     0,0600
  11.877        16299,9     93005,9     0,0600
  12.362        3645,6     21562,3     0,0600
  13.283        2150,1     12505,8     0,0600
  13.721        2088,4     12444,8     0,0600
  14.147        7096,5     40868,4     0,0600
  14.559        15208,5     90960,4     0,0600
  14.960        16078,5     96456,8     0,0600
  15.350        7581,7     45444,6     0,0600
  15.731        2201,8     13064,0     0,0600
  16.106        2884,6     16182,4     0,0600
  16.251         466,3      2779,5      0,0600
  16.470        2392,6     14353,5     0,0600
  16.828        1243,9      7257,0      0,0600
  17.177        2537,4     14692,0     0,0600
  17.520         491,6      2946,4      0,0600
  17.856        3441,9     19562,7     0,0600
```

Results :

Appears to be cubic I. (possible groups : Im3m, Im3, I23....).

ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
0.003	0.7976	18.8814	18.8814	18.8814	90.000	90.000	90.000
0.000	0.0000	0.0010	0.0010	0.0010	0.000	0.000	0.000
RECIPROCAL CELL :		0.05296	0.05296	0.05296	90.000	90.000	90.000
VOLUME (A**3) :		6731.364					

H	K	L	TH(OBS)	TH-ZERO	TH(CALC)	DIFF.
1	1	0	3.419	3.422	3.424	-0.001
2	0	0	4.839	4.842	4.842	0.000

2	1	1	5.929	5.932	5.932	0.001
3	1	0	7.656	7.659	7.660	-0.001
2	2	2	8.390	8.393	8.392	0.001
3	2	1	9.061	9.064	9.066	-0.002
4	0	0	9.690	9.693	9.693	0.000
3	3	0	10.280	10.283	10.283	0.000
3	3	2	11.369	11.372	11.372	0.001
4	2	2	11.877	11.880	11.879	0.001
5	1	0	12.362	12.365	12.366	-0.001
5	2	1	13.283	13.286	13.287	-0.001
4	4	0	13.721	13.724	13.725	-0.001
5	3	0	14.147	14.150	14.149	0.001
6	0	0	14.559	14.562	14.562	0.000
5	3	2	14.960	14.963	14.963	0.000
6	2	0	15.350	15.353	15.354	-0.001
5	4	1	15.731	15.734	15.736	-0.002
6	2	2	16.106	16.109	16.108	0.001
6	3	1	16.470	16.473	16.473	0.000
4	4	4	16.828	16.831	16.830	0.001
5	5	0	17.177	17.180	17.179	0.001
6	4	0	17.520	17.523	17.522	0.001
5	5	2	17.856	17.859	17.859	0.000

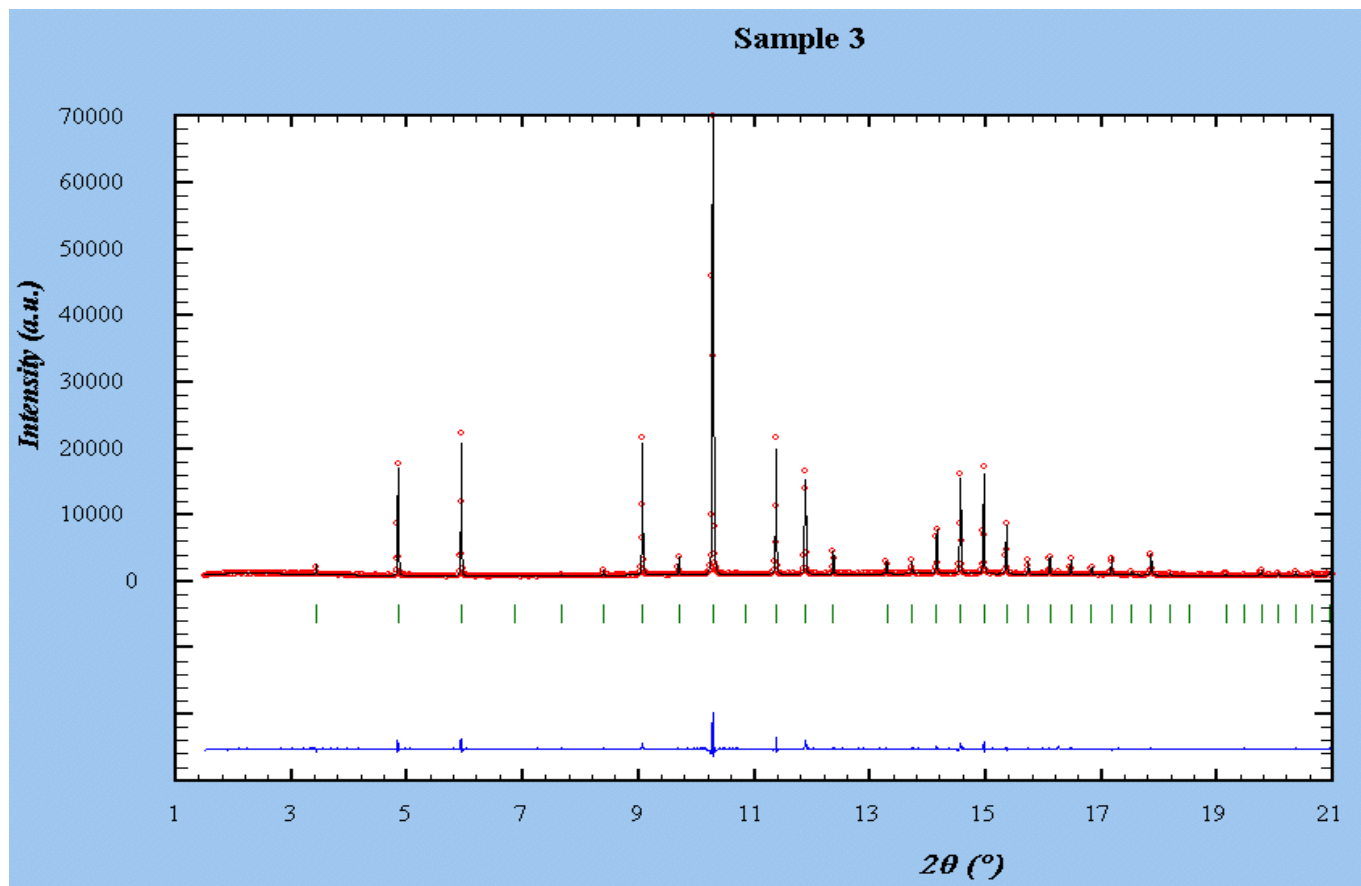
M(20) = 147.2846
F(20) = 498.6969 (7.4267632E-04, 54)

Final Rp on the .prf = 6.6828534E-02

FULLPROF

Cell confirmation and structure factors extraction (Le Bail fit).

Description in the space group Im3m :



SAMPLES 4 to 7

For these samples (as well as for sample 8), there is no structure determined. Without this ultimate proof that a cell is correct, we can only discuss about probable cells.

These samples have a long story. First attempts of solving the structures were made from conventional X-ray data. Only part of the cell parameters came from indexing attempts. Owing to the complexity of these cases, a proposal was deposited at the ESRF in 1998.

From conventional X-ray data :

Sample 4 (contains NaCl)

Monoclinic or triclinic, $a = 18.371(9) \text{ \AA}$, $c = 15.020(6) \text{ \AA}$, $\beta = 109.75(2)^\circ$

Sample 5

Orthorhombic or monoclinic, $a = 18.240(3) \text{ \AA}$, $b = 16.965(3) \text{ \AA}$, $\gamma = 90^\circ$

Sample 6

Monoclinic or triclinic, $a = 15.043(3) \text{ \AA}$, $c = 11.227(3) \text{ \AA}$, $\beta = 91.53(2)^\circ$

Sample 7

Monoclinic or triclinic, $a = 17.215(8) \text{ \AA}$, $c = 11.486(3) \text{ \AA}$, $\beta = 102.40(2)^\circ$

In the ESRF proposal, BM016 was expected, BM001 was obtained. The data were recorded in 1999. Extensive applications of a lot of indexing programs did not add anything to the above partial results. All these cases are characterized, more or less, by two long axis and a shorter third parameter difficult to determine.

At the IUCr Geneva meeting (XIXth Congress, 2002), optimistic declarations were made that some programs could cope with complex data, hence that Round Robin, requested by at least two participants speaking of indexing at a microsymposium about SDPD...

It was expected that light would come from these new algorithms and new experts.

Some results with various programs on conventional or synchrotron data are below. The problem is not that no solution is proposed. The problem is the overload of "solutions" having high figure of merit...

SAMPLE 4 with ITO :

Q (A)	Q (B)	Q (C)	Q (D)	Q (E)	Q (F)	LINES	FIGUR	LAT
						INDXD	MERIT	TYP
50.1	33.6	162.3	4.5	29.4	27.7	20.	145.0	P
50.1	33.6	162.2	11.7	36.5	27.7	20.	131.8	P
50.2	33.6	162.1	3.2	21.5	-27.7	20.	127.8	P
50.1	33.6	162.1	3.0	27.8	27.7	20.	122.7	P
50.1	33.5	655.1	25.2	27.6	27.7	20.	121.5	P
50.1	33.5	713.4	14.1	49.2	27.7	20.	105.4	P
50.1	33.5	702.8	25.2	20.1	-27.7	20.	105.4	P
50.1	713.4	33.5	14.1	27.7	0.0	20.	105.4	P
50.1	33.5	655.2	8.1	6.4	27.7	20.	87.0	P

THE DIRECT CONSTANTS OF THESE LATTICES

A	B	C	ALFA	BETA	GAMMA	VOLUME
15.2100	18.3493	7.9584	88.4750	99.3488	109.7512	2061.74
15.2778	18.3429	8.0187	90.6572	100.7991	109.2691	2077.18
15.1429	18.3821	7.9294	93.8110	97.7418	69.9218	2053.68
15.1931	18.3535	7.9552	88.0401	99.0192	109.8216	2060.63
15.0344	18.3860	3.9263	93.6169	92.9026	109.5203	1017.93
15.1282	18.3494	3.7762	90.1006	97.0117	109.6149	979.00
15.0719	18.4546	3.7992	96.1212	94.9775	69.8489	984.97
15.0171	3.7484	18.3710	92.7842	109.8036	89.0570	971.81
15.0184	18.3526	3.9084	91.2936	90.5102	109.7654	1013.37

SAMPLE 4 with DICVOL

MONOCLINIC SYSTEM

DIRECT PARAMETERS : A=34.6175 B= 8.7312 C=27.3482 BETA=124.808 VOLUME=6787.02
STANDARD DEVIATIONS : 0.0078 0.0064 0.0084 0.019

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
1	0	-1	26.51393	26.42297	0.09095	0.001420	0.00143	1.724	1.730	-0.006
2	0	-1	17.27602	17.25948	0.01654	0.003350	0.00336	2.646	2.649	-0.003
1	0	1	14.13118	14.12825	0.00292	0.005010	0.00501	3.235	3.236	-0.001
1	0	-2	13.37871	13.37099	0.00772	0.005590	0.00559	3.417	3.419	-0.002
3	0	-3	8.81000	8.80766	0.00235	0.012880	0.01289	5.190	5.191	-0.001
4	0	-2	8.63379	8.62974	0.00405	0.013420	0.01343	5.296	5.298	-0.002
0	0	3	7.48567	7.48493	0.00074	0.017850	0.01785	6.109	6.110	-0.001
2	0	2	7.06404	7.06413	-0.00008	0.020040	0.02004	6.474	6.474	0.000
5	0	-1	6.45917	6.45706	0.00211	0.023970	0.02398	7.081	7.083	-0.002
3	1	-3	6.19950	6.20075	-0.00126	0.026020	0.02601	7.378	7.377	0.001
4	0	1	5.87811	5.87797	0.00014	0.028940	0.02894	7.782	7.782	0.000
4	1	-3	5.83915	5.84141	-0.00226	0.029330	0.02931	7.834	7.831	0.003
6	0	-3	5.75553	5.75316	0.00237	0.030190	0.03021	7.948	7.951	-0.003
6	0	-2	5.67076	5.67699	-0.00622	0.031100	0.03103	8.067	8.058	0.009
4	0	-5	5.45606	5.45453	0.00154	0.033590	0.03361	8.385	8.387	-0.002
5	1	-3	5.34223	5.33909	0.00314	0.035040	0.03508	8.564	8.569	-0.005
1	0	4	4.99204	4.99220	-0.00015	0.040130	0.04013	9.166	9.166	0.000
5	1	-4		4.99878	-0.00674		0.04002		9.154	0.012
6	0	-5	4.96663	4.97028	-0.00366	0.040540	0.04048	9.213	9.206	0.007
1	0	-5	4.88671	4.88673	-0.00002	0.041880	0.04188	9.364	9.364	0.000
5	0	1		4.88695	-0.00023		0.04187		9.364	0.000
7	0	-2	4.79376	4.79229	0.00147	0.043520	0.04354	9.546	9.549	-0.003
3	0	3	4.70863	4.70942	-0.00079	0.045100	0.04509	9.719	9.717	0.002

* FIGURES OF MERIT

1.- M(21) = 13.9 (REF. 4)
2.- F(21) = 85.2(0.0026, 96) (REF. 5)

ORTHORHOMBIC SYSTEM

DIRECT PARAMETERS : A= 43.57299 B= 34.53791 C= 33.15367 VOLUME=49893.61
STANDARD DEVIATIONS : 0.02127 0.01397 0.04320

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
---	---	---	------	------	-----------	------	------	---------	---------	----------

1	0	1	26.51393	26.38455	0.12938	0.001420.00144	1.724	1.732	-0.008
0	2	0	17.27602	17.26895	0.00707	0.003350.00335	2.646	2.647	-0.001
1	1	2	14.13118	14.13628	-0.00510	0.005010.00500	3.235	3.234	0.001
3	1	0	13.37871	13.38862	-0.00991	0.005590.00558	3.417	3.414	0.003
3	0	3	8.81000	8.79485	0.01515	0.012880.01293	5.190	5.199	-0.009
4	1	2		8.80291	0.00709	0.01290		5.194	-0.004
0	4	0	8.63379	8.63448	-0.00068	0.013420.01341	5.296	5.296	0.000
0	2	4	7.48567	7.47231	0.01335	0.017850.01791	6.109	6.120	-0.011
2	3	3		7.48697	-0.00131	0.01784		6.108	0.001
2	2	4	7.06404	7.06814	-0.00410	0.020040.02002	6.474	6.470	0.004
4	2	3		7.07664	-0.01259	0.01997		6.462	0.012
2	5	1	6.45917	6.45840	0.00077	0.023970.02397	7.081	7.082	-0.001
0	2	5	6.19950	6.19011	0.00939	0.026020.02610	7.378	7.389	-0.011
6	2	2		6.20727	-0.00777	0.02595		7.369	0.009
5	3	3	5.87811	5.88231	-0.00420	0.028940.02890	7.782	7.776	0.006
3	5	2	5.83915	5.83834	0.00081	0.029330.02934	7.834	7.835	-0.001
0	6	0	5.75553	5.75632	-0.00079	0.030190.03018	7.948	7.947	0.001
6	3	2		5.75957	-0.00405	0.03015		7.942	0.006
7	2	1		5.76664	-0.01111	0.03007		7.933	0.015
0	3	5		5.74586	0.00967	0.03029		7.961	-0.013
2	4	4		5.76617	-0.01064	0.03008		7.933	0.015
4	5	1		5.74533	0.01020	0.03029		7.962	-0.014
5	4	2		5.75247	0.00306	0.03022		7.952	-0.004
7	1	2		5.74619	0.00934	0.03029		7.961	-0.013
0	6	1	5.67076	5.67147	-0.00070	0.031100.03109	8.067	8.066	0.001
4	0	5		5.66395	0.00682	0.03117		8.077	-0.010
5	2	4		5.67255	-0.00178	0.03108		8.064	0.003
0	1	6	5.45606	5.45622	-0.00016	0.033590.03359	8.385	8.385	0.000
6	0	4		5.46213	-0.00607	0.03352		8.376	0.009
3	3	5	5.34223	5.34296	-0.00073	0.035040.03503	8.564	8.563	0.001
3	6	0		5.35137	-0.00914	0.03492		8.549	0.015
5	5	1		5.34253	-0.00030	0.03504		8.564	0.000
7	4	1	4.99204	4.99182	0.00023	0.040130.04013	9.166	9.166	0.000
2	6	3	4.96663	4.97062	-0.00399	0.040540.04047	9.213	9.206	0.007
6	4	3		4.96522	0.00141	0.04056		9.216	-0.003
8	0	3	4.88671	4.88550	0.00122	0.041880.04190	9.364	9.366	-0.002
5	3	5	4.79376	4.79701	-0.00325	0.043520.04346	9.546	9.540	0.006
5	6	0		4.80309	-0.00933	0.04335		9.527	0.019
9	1	0		4.79457	-0.00081	0.04350		9.544	0.002
6	5	2		4.79142	0.00233	0.04356		9.551	-0.005
9	0	1		4.79063	0.00312	0.04357		9.552	-0.006
1	0	7	4.70863	4.70850	0.00012	0.045100.04511	9.719	9.719	0.000
3	3	6		4.71209					

* FIGURES OF MERIT

$$\begin{aligned} 1.- M(21) &= 5.0 && (\text{REF. 4}) \\ 2.- F(21) &= 27.1(0.0024, 329) && (\text{REF. 5}) \end{aligned}$$

SAMPLE 4 – some CRYSFIRE outputs :

FJZN v6.21a run started on 7Sep99 at 11:17:55

838ESRF = 838KM

10 solutions found with I20>15 and Merit > 7.0

I20 c	Merit alpha	Volume beta	V/V1 gamma	BL	IndexProg Q(A)	Date Q(B)	Time Q(C)	Pedig Q(D)	a Q(E)	b
Q(F)										
20	109.20	985.479	1.00	P	FJZNV6.21a	7Sep99	11:17:58	122	15.0662	18.4567
3.8019	96.229	94.843	69.867		50.1030	33.5429	701.8677	26.0593	18.9177	-
27.7320										

```

20  53.45  1955.892  1.98 P FJZNv6.21a  7Sep99 11:17:58  231  18.4149  29.4732
3.7727  93.504  94.861  73.616  32.1982  12.5260  708.7530  7.3374  21.2984  -
11.1824
20  12.06  17134.240  17.39 C FJZNv6.21a  7Sep99 11:17:58  111  36.2496  15.4435
31.7260  90.000  105.265  90.000  8.1770  41.9283  10.6750  .0000  4.9198
.0000
19  164.41  1958.215  1.99 I FJZNv6.21a  7Sep99 11:17:58  123  29.4183  3.7774
18.3477  90.000  106.172  90.000  12.5266  700.8289  32.2034  .0000  11.1878
.0000
19  149.18  979.041  .99 P FJZNv6.21a  7Sep99 11:17:58  121  15.1295  18.3478
3.7772  89.997  97.167  109.606  50.1090  33.5415  713.4016  13.8422  50.0768
27.7298
19  13.48  3897.230  3.95 B FJZNv6.21a  7Sep99 11:17:58  362  30.0167  36.6579
3.7685  92.833  92.769  70.309  12.5345  8.4051  706.6567  5.4342  6.3343  -
6.8845
19  9.57  1960.870  1.99 P FJZNv6.21a  7Sep99 11:17:58  233  18.4719  29.4373
3.7737  93.333  94.925  73.685  31.9866  12.5446  708.3058  6.7096  21.8412  -
11.1143
18  7.34  4259.686  4.32 P FJZNv6.21a  7Sep99 11:17:58  364  3.7588  36.7415
32.8121  109.785  92.582  89.126  709.2198  8.3663  10.5089  6.3420  7.3214
.0000
17  12.76  1870.895  1.90 P FJZNv6.21a  7Sep99 11:17:58  564  14.4398  34.5390
3.7825  92.125  96.773  87.774  48.6947  8.4043  709.5630  5.0579  43.3688  -
1.4053
16  8.51  2312.892  2.35 P FJZNv6.21a  7Sep99 11:17:58  551  35.0125  3.8250
17.6878  90.000  102.472  90.000  8.5566  683.5007  33.5271  .0000  7.3160
.0000
FJZN v6.21a run finished on 7Sep99 at 11:17:58 (Elapsed time: 3.63 sec)

```

SAMPLE 5 – some CRYSFIRE outputs :

```

FJZN v6.21a run started on 8Sep99 at 17:34:56
840court = 840court
8 solutions found with I20>15 and Merit > 7.0
I20  Merit  Volume  V/V1 BL IndexProg  Date  Time  Pedig  a  b
C  alpha  beta  gamma  Q(A)  Q(B)  Q(C)  Q(D)  Q(E)
Q(F)
20  45.06  961.403  1.00 P FJZNv6.21a  8Sep99 17:34:58  141  18.2616  16.9324
3.1133  90.000  92.926  90.000  30.0646  34.8789  1034.4390  .0000  18.0061
.0000
20  41.00  1040.071  1.08 P FJZNv6.21a  8Sep99 17:34:58  453  16.9608  18.2632
3.3694  93.211  93.534  89.802  34.8949  30.0754  886.9794  18.2642  21.6554
.0000
20  15.27  11179.970  11.63 C FJZNv6.21a  8Sep99 17:34:58  112  20.5689  29.8210
18.2267  90.000  90.000  90.000  23.6363  11.2449  30.1011  .0000  .0000
.0000
20  15.00  10826.270  11.26 C FJZNv6.21a  8Sep99 17:34:58  111  21.3421  27.8153
18.2371  90.000  90.000  90.000  21.9545  12.9250  30.0668  .0000  .0000
.0000
20  9.28  12930.940  13.45 P FJZNv6.21a  8Sep99 17:34:58  113  18.9901  37.3392
18.2364  90.000  90.000  90.000  27.7297  7.1725  30.0693  .0000  .0000
.0000
18  114.16  994.323  1.03 P FJZNv6.21a  8Sep99 17:34:58  551  16.9295  18.2338
3.2211  90.000  90.000  90.000  34.8911  30.0778  963.7951  .0000  .0000
.0000
16  13.61  689.887  .72 P FJZNv6.21a  8Sep99 17:34:58  261  9.0479  25.0063
3.1077  92.821  98.391  82.879  126.5785  16.2579  1059.0490  8.3231  103.3145  -
10.7230
16  7.73  1014.380  1.06 P FJZNv6.21a  8Sep99 17:34:58  451  16.6454  18.2549
3.3497  93.853  92.482  88.712  36.1739  30.1560  896.8635  21.8056  15.0944  -
1.2965
FJZN v6.21a run finished on 8Sep99 at 17:34:59 (Elapsed time: 2.30 sec)

```

Recent re-examinations with McMaille are below :

McMAILLE

SAMPLE 4

Which cell is the good one ?? Most lines are indexed as h0l lines.

```
=====
      FINAL LIST OF CELL PROPOSALS, sorted by Rp :
=====
```

Rp	Vol	Vol/V1	Ind	Nsol	a	b	c	alpha	beta	gamma
0.018	2891.701	1.00	19	1	19.3789	11.1609	15.0086	90.000	117.025	90.000
0.018	1002.139	0.35	19	1	15.0078	3.8682	19.3776	90.000	117.020	90.000
0.019	2273.531	0.79	19	1	18.3459	8.7747	15.0081	90.000	109.774	90.000
0.021	1506.862	0.52	19	1	15.0085	5.8159	18.3439	90.000	109.764	90.000
0.022	2707.739	0.94	20	2	19.3777	10.4520	15.0078	90.000	117.025	90.000
0.022	1636.860	0.57	19	2	19.3773	6.3182	15.0074	90.000	117.015	90.000
0.023	1627.970	0.56	19	1	15.0085	6.2829	19.3776	90.000	117.008	90.000
0.023	2819.319	0.97	19	3	19.3781	10.8829	15.0076	90.000	117.027	90.000
0.023	2546.214	0.88	19	2	18.3465	9.8268	15.0087	90.000	109.781	90.000
0.023	2746.090	0.95	19	1	15.0086	10.5994	18.3421	90.000	109.760	90.000
0.024	2457.777	0.85	19	2	19.3793	9.4869	15.0079	90.000	117.031	90.000
0.024	2444.901	0.85	19	1	18.3439	9.4368	15.0090	90.000	109.778	90.000
0.024	2760.239	0.95	19	1	19.3787	10.6523	15.0084	90.000	117.010	90.000
0.025	2936.511	1.02	19	2	18.3421	11.3355	15.0076	90.000	109.764	90.000
0.025	1443.794	0.50	19	1	15.0069	5.5730	19.3794	90.000	117.024	90.000
0.025	2066.479	0.71	19	1	18.3454	7.9759	15.0070	90.000	109.766	90.000
0.026	2281.105	0.79	19	1	15.0077	8.8056	18.3427	90.000	109.773	90.000
0.026	1576.654	0.55	19	1	18.3452	6.0850	15.0094	90.000	109.780	90.000
0.026	1660.620	0.57	20	1	18.3472	6.4085	15.0093	90.000	109.784	90.000
0.026	2317.412	0.80	19	1	18.3469	8.9440	15.0079	90.000	109.781	90.000
0.026	1838.071	0.64	19	1	18.3472	7.0939	15.0076	90.000	109.777	90.000
0.027	2444.688	0.85	19	1	15.0082	9.4365	18.3441	90.000	109.781	90.000
0.027	1110.475	0.38	19	1	15.0084	4.2854	19.3785	90.000	117.005	90.000
0.027	875.048	0.30	19	1	18.3463	3.3773	15.0088	90.000	109.786	90.000
0.027	1237.548	0.43	19	1	18.3442	4.7766	15.0091	90.000	109.781	90.000
0.028	1014.544	0.35	19	1	15.0094	3.9154	19.3771	90.000	117.010	90.000
0.028	753.979	0.26	19	1	15.0080	2.9104	19.3795	90.000	117.035	90.000
0.028	2641.566	0.91	19	1	15.0098	10.1949	19.3781	90.000	117.023	90.000
0.029	2509.448	0.87	19	1	18.3443	9.6849	15.0086	90.000	109.762	90.000
0.029	1164.875	0.40	19	1	15.0087	4.4961	19.3800	90.000	117.036	90.000
0.029	957.295	0.33	19	1	19.3794	3.6945	15.0076	90.000	117.010	90.000
0.029	2547.138	0.88	19	1	15.0083	9.8325	18.3424	90.000	109.777	90.000
0.030	1368.346	0.47	19	1	18.3410	5.2823	15.0070	90.000	109.756	90.000
0.030	1138.097	0.39	19	1	15.0097	4.3925	19.3765	90.000	117.015	90.000
0.030	2360.000	0.82	19	1	15.0070	9.1107	18.3412	90.000	109.761	90.000
0.031	1818.669	0.63	19	1	18.3409	7.0210	15.0064	90.000	109.754	90.000
0.031	1528.014	0.53	19	1	19.3781	5.8976	15.0097	90.000	117.029	90.000
0.031	2827.793	0.98	19	1	18.3447	10.9137	15.0099	90.000	109.781	90.000
0.031	1250.184	0.43	19	1	19.3804	4.8251	15.0075	90.000	117.023	90.000
0.031	1680.236	0.58	20	1	15.0056	6.4869	19.3784	90.000	117.030	90.000

0.031	1921.285	0.66	20	1	18.3456	7.4159	15.0061	90.000	109.766	90.000
0.032	2032.725	0.70	19	2	19.3773	7.8449	15.0080	90.000	117.001	90.000
0.032	1355.202	0.47	19	1	15.0079	5.2298	18.3484	90.000	109.776	90.000
0.032	1938.442	0.67	19	2	19.3791	7.4842	15.0046	90.000	117.034	90.000
0.032	1900.907	0.66	19	1	19.3780	7.3387	15.0062	90.000	117.030	90.000
0.032	2702.747	0.93	20	2	15.0064	10.4320	18.3464	90.000	109.773	90.000
0.033	2824.891	0.98	19	1	15.0065	10.9038	19.3804	90.000	117.025	90.000
0.033	1118.176	0.39	19	2	18.3413	4.3167	15.0078	90.000	109.770	90.000
0.033	2207.627	0.76	19	1	15.0075	8.5223	18.3427	90.000	109.776	90.000
0.033	1141.737	0.39	19	1	18.3434	4.4063	15.0100	90.000	109.763	90.000
0.034	1870.686	0.65	19	1	15.0100	7.2193	18.3439	90.000	109.765	90.000
0.035	1941.449	0.67	19	2	18.3417	7.4935	15.0085	90.000	109.752	90.000
0.035	1830.109	0.63	19	2	19.3781	7.0655	15.0057	90.000	117.029	90.000
0.035	1679.458	0.58	20	1	18.3395	6.4836	15.0071	90.000	109.750	90.000
0.037	728.350	0.25	19	1	15.0092	2.8115	18.3406	90.000	109.766	90.000
0.037	2842.678	0.98	19	1	15.0091	10.9730	18.3431	90.000	109.785	90.000
0.038	1974.237	0.68	19	1	15.0071	7.6206	18.3458	90.000	109.784	90.000
0.039	2766.307	0.96	19	1	18.3440	10.6781	15.0089	90.000	109.789	90.000
0.040	1107.677	0.38	19	1	15.0077	4.2764	18.3406	90.000	109.773	90.000
0.041	1255.954	0.43	19	1	15.0068	4.8472	18.3488	90.000	109.780	90.000
0.042	2550.795	0.88	19	1	15.0071	9.8476	19.3746	90.000	117.017	90.000
0.043	2503.647	0.87	19	1	19.3811	9.6639	15.0083	90.000	117.045	90.000
0.044	732.713	0.25	19	1	19.3797	2.8271	15.0089	90.000	116.998	90.000
0.046	982.226	0.34	19	1	18.3385	3.7924	15.0063	90.000	109.753	90.000
0.047	1309.300	0.45	19	1	18.3401	5.0539	15.0100	90.000	109.766	90.000
0.048	2403.691	0.83	20	1	18.3480	9.2754	15.0080	90.000	109.763	90.000
0.050	1053.292	0.36	19	1	15.0079	4.0649	18.3447	90.000	109.751	90.000
0.053	2395.586	0.83	19	1	15.0090	9.2458	19.3830	90.000	117.048	90.000
0.058	2497.476	0.86	19	1	15.0041	9.6423	19.3764	90.000	117.011	90.000
0.070	2949.156	1.02	19	1	15.0120	11.3815	19.3721	90.000	117.000	90.000
0.220	2542.303	0.88	16	1	10.4282	14.1229	17.2677	90.000	91.450	90.000
0.290	2601.947	0.90	16	1	14.4877	10.4037	17.7088	90.000	102.887	90.000
0.424	2906.684	1.01	16	1	19.2461	11.2917	15.0034	90.000	116.942	90.000

"Best" cell :

ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
0.000	0.7978	19.3770	11.1549	15.0084	90.000	117.021	90.000
0.000	0.0000	0.0011	0.0040	0.0008	0.000	0.002	0.000
RECIPROCAL CELL :		0.05793	0.08965	0.07479	90.000	62.979	90.000
VOLUME (A**3) :		2889.904					

H	K	L	TH(OBS)	TH-ZERO	TH(CALC)	DIFF.
1	0	0	2.648	2.648	2.648	0.000
1	0	-1	3.237	3.237	3.237	0.000
0	0	1	3.419	3.419	3.419	0.000
2	0	0	5.298	5.298	5.298	0.000
1	0	-2	6.111	6.111	6.111	0.000
2	0	-2	6.476	6.476	6.476	0.000
3	0	-1	7.083	7.083	7.084	-0.001
3	0	-2	7.784	7.784	7.784	0.000
3	0	0	7.950	7.950	7.950	0.000
1	0	2	8.387	8.387	8.387	0.000
2	0	-3	9.168	9.168	9.168	0.000
1	0	-3	9.366	9.366	9.366	0.000
4	0	-1	9.548	9.548	9.549	-0.001
3	0	-3	9.721	9.721	9.721	0.001
0	0	3	10.270	10.270	10.270	0.000
4	1	-1	10.395	10.395	10.395	0.000
4	0	0	10.608	10.608	10.607	0.001
4	0	-3	10.910	10.910	10.910	0.000
1	0	3	11.719	11.719	11.720	-0.001

M(20) = 188.8355
 F(20) = 970.8089 (3.2700598E-04, 63)

SAMPLE 5

Could be the good cell ??

=====

FINAL LIST OF CELL PROPOSALS, sorted by Rp :

=====

Rp	Vol	Vol/V1	Ind	Nsol	a	b	c	alpha	beta	gamma
0.126	1857.174	1.00	38	1	6.0160	18.2330	17.7632	90.000	107.606	90.000

ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
0.003	0.7976	6.0125	18.2334	17.7529	90.000	107.602	90.000
0.004	0.0000	0.0029	0.0088	0.0087	0.000	0.022	0.000
RECIPROCAL CELL :		0.17449	0.05484	0.05910	90.000	72.398	90.000
VOLUME (A**3) :		1855.098					

0	H	K	L	TH(OBS)	TH-ZERO	TH(CALC)	DIFF.
	0	1	1	3.683	3.686	3.685	0.000
	0	2	0	5.013	5.016	5.015	0.001
	0	0	2	5.401	5.404	5.403	0.000
	0	2	1	5.695	5.698	5.697	0.001
	0	1	2	5.954	5.957	5.957	-0.001
	0	2	2	7.372	7.375	7.374	0.000
	1	0	-1	7.612	7.615	7.612	0.002
	0	3	1	7.995	7.998	7.996	0.001
	1	1	0	8.365	8.368	8.366	0.001
	0	1	3	8.485	8.488	8.489	-0.001
	1	2	-1	9.122	9.125	9.119	0.005
	1	0	1	9.169	9.172	9.170	0.001
	0	3	2	9.268	9.271	9.268	0.002
	1	2	0	9.428	9.431	9.430	0.001
	1	1	1	9.504	9.507	9.508	-0.001
	1	2	-2	9.594	9.597	9.595	0.002
	1	1	-3	9.827	9.830	9.833	-0.003
	0	4	0	10.038	10.041	10.039	0.002
	1	2	1	10.454	10.457	10.457	0.000
	1	3	-1	10.714	10.717	10.711	0.005
	1	2	-3	10.742	10.745	10.753	-0.009
	0	0	4	10.811	10.814	10.819	-0.006
	1	0	2	10.925	10.928	10.917	0.011
	1	3	0	10.944	10.947	10.977	-0.031
	0	3	3	11.070	11.073	11.071	0.001
	1	3	-2	11.119	11.122	11.120	0.002
	0	4	2	11.405	11.408	11.407	0.000
	1	3	1	11.871	11.874	11.872	0.001
	0	2	4	11.927	11.930	11.931	-0.001
	1	3	-3	12.130	12.133	12.135	-0.002
	1	4	-1	12.613	12.616	12.610	0.005
	1	4	0	12.837	12.840	12.837	0.002
	0	4	3	12.915	12.918	12.918	0.000
	1	0	3	12.999	13.002	13.001	0.000
	1	3	2	13.268	13.271	13.272	-0.001
	1	3	-4	13.627	13.630	13.624	0.006
	1	1	-5	13.713	13.716	13.711	0.004
	1	4	-3	13.840	13.843	13.842	0.000

Final M(20) = 120.4281

SAMPLE 7

=====

FINAL LIST OF CELL PROPOSALS, sorted by Rp :

=====

Rp	Vol	Vol/V1	Ind	Nsol	a	b	c	alpha	beta	gamma
0.119	1928.557	1.00	16	1	18.5051	10.1475	11.3831	90.000	115.546	90.000
0.120	2381.732	1.23	16	1	11.3837	12.5327	18.5017	90.000	115.537	90.000
0.124	1040.333	0.54	16	1	11.3835	5.4727	17.0448	90.000	101.560	90.000
0.127	1905.568	0.99	17	1	18.5116	10.0247	11.3830	90.000	115.565	90.000

Etc

Almost exclusively h0l refections in these proposals. One example below :

ZERO	LAMBDA	A	B	C	ALPHA	BETA	GAMMA
-0.001	0.7978	18.5182	10.1398	11.3812	90.000	115.578	90.000
0.003	0.0000	0.0088	0.0049	0.0056	0.000	0.023	0.000

RECIPROCAL CELL : 0.05987 0.09862 0.09741 90.000 64.422 90.000

VOLUME (A**3) : 1927.618

H	K	L	TH(OBS)	TH-ZERO	TH(CALC)	DIFF.
1	0	0	2.739	2.738	2.737	0.002
1	0	-1	4.102	4.101	4.099	0.003
0	0	1	4.450	4.449	4.454	-0.004
2	0	-1	5.360	5.359	5.363	-0.003
2	0	0	5.476	5.475	5.475	0.000
1	0	1	6.152	6.151	6.154	-0.003
1	0	-2	8.119	8.118	8.115	0.003
2	0	-2	8.203	8.202	8.203	0.000
2	0	1	8.430	8.429	8.423	0.006
4	0	-1	9.890	9.889	9.889	0.000
4	0	0	10.962	10.961	10.963	-0.001
4	1	-2	11.652	11.651	11.650	0.001
3	2	-1	11.729	11.728	11.723	0.006
2	0	-3	12.073	12.072	12.074	-0.002
3	2	0	12.211	12.210	12.216	-0.006
3	0	-3	12.318	12.317	12.317	0.000

M(20) = 44.14456

F(20) = 197.0437 (2.0300071E-03, 50)

SAMPLE 8

This sample is characterized probably by the same problem as samples 4-7. After zeropoint correction, indexing proposes tetragonal or hexagonal or orthorhombic cells having in common two parameters close to 28.9 and 9.37 Å.

TREOR : mostly h0l lines

```

TOTAL NUMBER OF LINES = 34
A = 9.377719 .000298 A ALFA = 90.000000 .000000 DEG
B = 9.377719 .000298 A BETA = 90.000000 .000000 DEG
C = 28.931856 .001131 A GAMMA = 90.000000 .000000 DEG
UNIT CELL VOLUME = 2544.31 A**3
  H  K  L SST-OBS  SST-CALC  DELTA  2TH-OBS  2TH-CALC  D-OBS  FREE PARAM.
  1  0  0 .006758 .006747 .000011  9.431  9.423  9.3699
  1  0  2 .009580 .009582 -.000002 11.234 11.235  7.8698
  0  0  4 .011360 .011341 .000019 12.237 12.227  7.2269
  1  0  3 .013139 .013126 .000013 13.164 13.158  6.7200
  1  0  5 .024477 .024468 .000009 18.002 17.999  4.9234
  2  0  1 .027703 .027696 .000007 19.162 19.160  4.6279
  1  0  6 .032278 .032265 .000013 20.700 20.696  4.2874
  2  0  3 .033360 .033367 -.000007 21.048 21.050  4.2173
  2  0  4 .038321 .038329 -.000008 22.578 22.580  3.9349
  0  0  8 .045393 .045365 .000027 24.603 24.595  3.6154
  2  0  7 .061725 .061720 .000004 28.771 28.770  3.1004
  3  0  2 .063565 .063557 .000007 29.206 29.204  3.0552
  1  0  9 .064183 .064162 .000021 29.351 29.346  3.0404
  3  0  4 .072092 .072063 .000029 31.150 31.144  2.8688
  3  0  5 .078492 .078443 .000049 32.540 32.530  2.7494
  3  0  7 .095461 .095455 .000006 35.994 35.993  2.4931
  0  0 12 .102110 .102072 .000038 37.271 37.264  2.4105
  3  1  7 .102202 .102202 .000000 37.288 37.288  2.3651
  3  0  8 .106070 .106087 -.000017 38.014 38.017  2.3443
  4  0  0 .107958 .107950 .000008 38.364 38.362  38.493
  4  0  1 .108659 .108659 .000000 38.526 38.523  2.3349
  1  0 12 .108837 .108819 .000018 38.878 38.883  2.3145
  4  0  2 .110758 .110785 -.000027 39.246 39.241  2.2937
  2  0 11 .112782 .112756 .000025 39.527 39.526  2.2780
  3  1  8 .114338 .114330 .000008 40.203 40.206  2.2412
  4  0  3 .118119 .118137 -.000019 40.410 40.411  2.2302
  3  0  9 .119287 .119291 -.000004 41.526 41.526  2.1728
  4  0  4 .125673 .125671 .000002 41.681 41.676  2.1651
  4  0  5 .126571 .126540 .000031 42.103 42.108  2.1444
  1  0 13 .129030 .129060 -.000030 42.539 42.541  2.1234
  2  0 12 .131591 .131605 -.000014 44.385 44.387  2.0393
  4  0  7 .142672 .142683 -.000011 44.881 44.875  2.0179
  1  0 14 .145713 .145678 .000035 46.095 46.090  1.9675
  3  1 11 .153268 .153238 .000030 46.103 46.103  1.8913
  4  0  8 .165869 .165919 -.000050 48.931 48.930  1.8599
  2  0 14 .171516 .171507 .000009 48.931 48.930  1.8599
  5  0  2 .171516 .171507 .000009 48.931 48.930  1.8599
NUMBER OF OBS. LINES = 34
NUMBER OF CALC. LINES = 38
M( 20)= 37 AV.EPS.= .0000157
F 20 = 49.( .004436, 93)
M( 30)= 33 AV.EPS.= .0000162
F 30 = 57.( .003954, 135)
M( 34)= 29 AV.EPS.= .0000179
F 34 = 51.( .004059, 166)
M CF. J.APPL.CRYST. 1(1968)108
F CF. J.APPL.CRYST. 12(1979)60

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0 LINES ARE UNINDEXED

Some series of CRYSFIRE outputs on different patterns

Running summary of all solutions logged so far for this dataset name,
sorted in descending order of I20 then Merit (as defined by each program)

120	Merit	Volume	V/V1	BL	Index	Prog	Date	Time	Pedig	a	b
c	alpha	beta	gamma		Q(A)	Q(B)	Q(C)	Q(D)	Q(E)		
Q(F)	Description (up to 80-chars, from Run-Title line)										
20	51.7	743.516	1.00	P	DICVOL91/log	20Mar01	14:17:15	Mon__4	9.4000	28.9313	
2.7405	90.000	93.955	90.000		113.714	11.947	1337.862	.000	53.805		
.000	rb7 = (No title provided yet)										
20	51.7	742.839	1.00	P	DICVOL91/log	20Mar01	14:17:15	Mon__3	9.3915	28.9313	
2.7380	90.000	93.114	90.000		113.714	11.947	1337.878	.000	42.377		
.000	rb7 = (No title provided yet)										
20	51.5	742.798	1.00	P	DICVOL91/log	20Mar01	14:17:15	Mon__2	9.3911	28.9309	
2.7380	90.000	93.112	90.000		113.723	11.947	1337.873	.000	42.351		
.000	rb7 = (No title provided yet)										
20	51.0	744.330	1.00	P	DICVOL91/log	20Mar01	14:17:15	Mon_15	9.4105	28.9313	
2.7435	90.000	94.791	90.000		113.714	11.947	1337.920	.000	65.155		
.000	rb7 = (No title provided yet)										
20	50.8	742.234	1.00	P	DICVOL91/log	20Mar01	14:17:15	Mon_10	28.9765	9.3773	
2.7359	90.000	93.213	90.000		11.947	113.722	1340.189	.000	14.184		
.000	rb7 = (No title provided yet)										
20	50.7	742.234	1.00	P	DICVOL91/log	20Mar01	14:17:15	Mon__8	28.9523	9.3773	
2.7359	90.000	92.201	90.000		11.947	113.722	1337.952	.000	9.711		
.000	rb7 = (No title provided yet)										
20	50.6	773.545	1.04	P	DICVOL91/log	20Mar01	14:17:15	Ort__1	28.9336	9.3777	
2.8509	90.000	90.000	90.000		11.945	113.712	1230.354	.000	.000		
.000	rb7 = (No title provided yet)										
20	50.2	755.533	1.02	P	DICVOL91/log	20Mar01	14:17:15	Mon__1	9.3800	28.9313	
2.7848	90.000	91.299	90.000		113.715	11.947	1290.135	.000	17.366		
.000	rb7 = (No title provided yet)										
20	49.5	757.111	1.02	P	DICVOL91/log	20Mar01	14:17:15	Mon_20	9.5292	28.9313	
2.7906	90.000	100.232	90.000		113.713	11.947	1325.957	.000	137.952		
.000	rb7 = (No title provided yet)										
20	49.5	757.110	1.02	P	DICVOL91/log	20Mar01	14:17:15	Mon_17	9.4417	28.9313	
2.7906	90.000	96.678	90.000		113.714	11.947	1301.721	.000	89.482		
.000	rb7 = (No title provided yet)										
20	48.7	770.019	1.04	P	DICVOL91/log	20Mar01	14:17:15	Mon_21	9.4288	28.9313	
2.8382	90.000	95.975	90.000		113.715	11.947	1255.005	.000	78.648		
.000	rb7 = (No title provided yet)										
20	48.5	748.012	1.01	P	DICVOL91/log	20Mar01	14:17:15	Mon_26	29.1769	9.3773	
2.7											

20	46.5	756.802	1.02	P	DICVOL91/log	20Mar01	14:17:15	Mon__7	28.9324	9.3773
2.7896	90.000	90.574	90.000	11.947	113.722	1285.168	.000	2.483		
.000 rb7 = (No title provided yet)										
20	46.5	756.802	1.02	P	DICVOL91/log	20Mar01	14:17:15	Mon_23	29.0387	9.3773
2.7896	90.000	94.938	90.000	11.947	113.722	1294.631	.000	21.411		
.000 rb7 = (No title provided yet)										
20	46.5	756.800	1.02	P	DICVOL91/log	20Mar01	14:17:15	Mon_24	29.0943	9.3773
2.7896	90.000	96.076	90.000	11.948	113.722	1299.599	.000	26.379		
.000 rb7 = (No title provided yet)										
20	46.2	748.957	1.01	P	DICVOL91/log	20Mar01	14:17:15	Mon_19	9.4899	28.9337
2.7603	90.000	98.819	90.000	113.712	11.945	1344.056	.000	119.873		
.000 rb7 = (No title provided yet)										
20	46.2	748.954	1.01	P	DICVOL91/log	20Mar01	14:17:15	Mon_18	9.4681	28.9337
2.7603	90.000	97.925	90.000	113.713	11.945	1337.897	.000	107.557		
.000 rb7 = (No title provided yet)										
20	45.5	770.067	1.04	P	DICVOL91/log	20Mar01	14:17:15	Mon_22	9.4290	28.9337
2.8381	90.000	95.979	90.000	113.712	11.945	1255.112	.000	78.703		
.000 rb7 = (No title provided yet)										
20	43.4	770.987	1.04	P	DICVOL91/log	20Mar01	14:17:15	Mon_12	28.9351	9.3775
2.8416	90.000	90.647	90.000	11.946	113.717	1238.596	.000	2.747		
.000 rb7 = (No title provided yet)										
20	43.3	742.103	1.00	P	DICVOL91/log	20Mar01	14:17:15	Mon_25	29.2468	9.3776
2.7353	90.000	98.424	90.000	11.947	113.715	1365.879	.000	37.428		
.000 rb7 = (No title provided yet)										
20	42.80	2324.858	3.13	B	KOHLv6.20h	20Mar01	14:22:53	63	18.7564	28.9308
4.2844	90.000	90.000	90.000	28.4249	11.9476	544.7896	.0000	.0000		
.0000 rb7 = (No title provided yet)										
20	42.4	768.763	1.03	P	DICVOL91/log	20Mar01	14:17:15	Mon_13	28.9405	9.3777
2.8333	90.000	91.245	90.000	11.945	113.712	1246.292	.000	5.302		
.000 rb7 = (No title provided yet)										
20	40.7	775.611	1.04	P	DICVOL91/log	20Mar01	14:17:15	Mon_14	29.0160	9.3776
2.8588	90.000	94.378	90.000	11.947	113.715	1230.752	.000	18.513		
.000 rb7 = (No title provided yet)										
20	38.0	773.521	1.04	P	DICVOL91/log	20Mar01	14:17:15	Mon__6	28.9354	2.8510
9.3766	90.000	90.015	90.000	11.944	1230.284	113.739	.000	.019		
.000 rb7 = (No title provided yet)										
20	35.3	747.877	1.01	P	DICVOL91/log	20Mar01	14:17:15	Mon_27	29.2832	9.3773
2.7567	90.000	98.896	90.000	11.947	113.722	1348.134	.000	39.252		
.000 rb7 = (No title provided yet)										
20	32.13	1555.863	2.09	P	LZONv6.22g	20Mar01	14:35:30	50078	28.9536	9.3791
5.7351	90.000	92.561	90.000	11.9526	113.6773	304.6422	.0000	5.3931		
.0000 rb7 = (No title provided yet)										
20	31.22	3042.219	4.09	B	KOHLv6.20h	20Mar01	14:22:53	45	18.7562	28.9321
5.6062	90.000	90.000	90.000	28.4257	11.9465	318.1750	.0000	.0000		
.0000 rb7 = (No title provided yet)										
20	30.66	1613.157	2.17	P	LZONv6.22g	20Mar01	14:35:30	50085	29.0093	9.3779
5.9469	90.000	94.350	90.000	11.9517	113.7083	284.4001	.0000	8.8449		
.0000 rb7 = (No title provided yet)										
20	26.41	3246.717	4.37	B	KOHLv6.20h	20Mar01	14:22:53	41	18.7529	28.9306
5.9844	90.000	90.000	90.000	28.4357	11.9477	279.2296	.0000	.0000		
.0000 rb7 = (No title provided yet)										
20	25.97	3124.509	4.20	C	LZONv6.22g	20Mar01	14:35:30	50003	5.7584	57.8638
9.3776	90.000	89.538	90.000	301.5996	2.9867	113.7227	.0000	-2.9840		
.0000 rb7 = (No title provided yet)										
20	25.56	2439.930	3.28	P	LZONv6.22g	20Mar01	14:35:30	60511	10.2388	28.9263
8.9932	90.000	113.644	90.000	113.6738	11.9513	147.3426	.0000	103.8075		
.0000 rb7 = (No title provided yet)										
20	25.27	1395.675	1.88	P	LZONv6.22g	20Mar01	14:35:30	50067	9.4076	28.9843
5.1446	93.611	94.513	89.716	113.6936	11.9509	381.6870	8.4816	32.7179		
.0000 rb7 = (No title provided yet)										
20	24.75	1554.661	2.09	P	KOHLv6.20h	20Mar01	14:22:53	68	9.3807	28.9271
5.7292	90.000	90.000	90.000	113.6391	11.9506	304.6564	.0000	.0000		
.0000 rb7 = (No title provided yet)										

20	23.44	5089.489	6.85	B	KOHLv6.20h	20Mar01	14:22:53	6	13.3396	28.9262
13.1898	90.000	90.000	90.000	56.1968		11.9514	57.4807	.0000	.0000	
.0000 rb7 = (No title provided yet)										
20	23.05	3475.901	4.67	P	KOHLv6.20h	20Mar01	14:22:53	36	18.7552	28.9273
6.4068	90.000	90.000	90.000	28.4288		11.9505	243.6254	.0000	.0000	
.0000 rb7 = (No title provided yet)										
20	21.8	3544.92	4.77	B	IT012/log	20Mar01	14:15:47	152	19.0186	28.9662
6.5318	92.857	99.467	89.530	28.415		11.948	241.489	5.282	27.219	
.000 rb7 = (No title provided yet)										
20	21.60	3581.783	4.82	B	LZONv6.22g	20Mar01	14:35:30	60818	11.5298	28.9234
11.4104	90.000	109.730	90.000	84.8991		11.9537	86.6853	.0000	57.9216	
.0000 rb7 = (No title provided yet)										
20	21.35	4465.494	6.01	A	LZONv6.22g	20Mar01	14:35:30	60136	9.9675	57.8474
8.2299	90.000	70.226	90.000	113.6634		2.9884	166.7237	.0000	-93.1447	
.0000 rb7 = (No title provided yet)										
20	20.93	4218.947	5.67	P	KOHLv6.20h	20Mar01	14:22:53	20	15.5517	28.9292
9.3775	90.000	90.000	90.000	41.3470		11.9489	113.7159	.0000	.0000	
.0000 rb7 = (No title provided yet)										
20	20.71	3833.601	5.16	B	LZONv6.22g	20Mar01	14:35:30	50074	13.7158	29.3974
10.2436	94.107	109.392	97.481	61.3868		11.9510	108.7487	8.8539	56.4047	
8.8653 rb7 = (No title provided yet)										
20	20.64	3316.278	4.46	P	KOHLv6.20h	20Mar01	14:22:53	39	12.2229	28.9253
9.3799	90.000	90.000	90.000	66.9344		11.9521	113.6592	.0000	.0000	
.0000 rb7 = (No title provided yet)										
20	20.44	3225.671	4.34	B	LZONv6.22g	20Mar01	14:35:30	60746	11.2924	29.1246
10.9223	93.380	115.316	93.674	96.9159		11.9472	103.5308	6.7332	86.7521	
6.7336 rb7 = (No title provided yet)										
20	20.36	3897.358	5.24	B	LZONv6.22g	20Mar01	14:35:30	60879	12.3927	29.0470
11.2785	92.889	105.436	93.397	70.4791		11.9504	85.0091	4.3832	41.7922	
4.3809 rb7 = (No title provided yet)										
20	20.16	2921.395	3.93	P	KOHLv6.20h	20Mar01	14:22:53	46	10.7685	28.9249
9.3792	90.000	90.000	90.000	86.2366		11.9524	113.6768	.0000	.0000	
.0000 rb7 = (No title provided yet)										
20	20.15	2435.481	3.28	P	KOHLv6.20h	20Mar01	14:22:53	60	9.3791	28.9247
8.9775	90.000	90.000	90.000	113.6777		11.9526	124.0777	.0000	.0000	
.0000 rb7 = (No title provided yet)										

I20	Merit	Volume	V/V1	BL	IndexProg	Date	Time	Pedig	a	b
c	alpha	beta	gamma	Q(A)	Q(B)	Q(C)	Q(D)	Q(E)		
Q(F) Description (up to 80-chars, from Run-Title line)										
20	55.64	773.475	1.00	P	LOSHv6.1a	20Mar01	17:11:56	1	9.3779	28.9308
2.8509	90.000	90.000	90.000	113.7078	11.9476	1230.3740	.0000	.0000		
.0000 rb72 = (No title provided yet)										
20	52.02	3524.816	4.56	F	LOSHv6.1a	20Mar01	17:11:56	247	18.7559	57.8617
3.2479	90.000	90.000	90.000	28.4265	2.9869	947.9524	.0000	.0000		
.0000 rb72 = (No title provided yet)										
20	51.9	773.523	1.00	P	DICVOL91/log	20Mar01	16:51:32	Ort__1	28.9331	9.3776
2.8509	90.000	90.000	90.000	11.946	113.715	1230.345	.000	.000		
.000 rb72 = (No title provided yet)										
20	51.6	742.827	.96	P	DICVOL91/log	20Mar01	16:51:32	Mon__6	9.3914	28.9311
2.7380	90.000	93.113	90.000	113.716	11.947	1337.876	.000	42.363		
.000 rb72 = (No title provided yet)										
20	50.9	744.314	.96	P	DICVOL91/log	20Mar01	16:51:32	Mon_26	9.4104	28.9310
2.7435	90.000	94.791	90.000	113.717	11.947	1337.920	.000	65.156		
.000 rb72 = (No title provided yet)										
20	50.4	757.110	.98	P	DICVOL91/log	20Mar01	16:51:32	Mon_28	9.4416	28.9316
2.7906	90.000	96.678	90.000	113.716	11.947	1301.721	.000	89.483		
.000 rb72 = (No title provided yet)										
20	50.3	755.517	.98	P	DICVOL91/log	20Mar01	16:51:32	Mon__1	9.3799	28.9310
2.7848	90.000	91.299	90.000	113.717	11.947	1290.135	.000	17.366		
.000 rb72 = (No title provided yet)										

20	50.2	743.906	.96	P	DICVOL91/log	20Mar01	16:51:32	Mon__8	9.4051	28.9312
2.7420	90.000	94.396	90.000	113.719	11.947	1337.901	.000	59.795		
.000 rb72 = (No title provided yet)										
20	50.2	742.844	.96	P	DICVOL91/log	20Mar01	16:51:32	Mon__3	9.3914	28.9318
2.7380	90.000	93.114	90.000	113.716	11.947	1337.878	.000	42.377		
.000 rb72 = (No title provided yet)										
20	50.1	743.516	.96	P	DICVOL91/log	20Mar01	16:51:32	Mon__7	9.3999	28.9316
2.7405	90.000	93.955	90.000	113.717	11.947	1337.862	.000	53.806		
.000 rb72 = (No title provided yet)										
20	49.2	775.538	1.00	P	DICVOL91/log	20Mar01	16:51:32	Mon_10	9.4017	28.9310
2.8586	90.000	94.113	90.000	113.717	11.947	1230.079	.000	53.650		
.000 rb72 = (No title provided yet)										
20	49.2	773.590	1.00	P	DICVOL91/log	20Mar01	16:51:32	Mon__4	9.3778	28.9311
2.8514	90.000	90.449	90.000	113.717	11.947	1230.015	.000	5.862		
.000 rb72 = (No title provided yet)										
20	49.0	755.538	.98	P	DICVOL91/log	20Mar01	16:51:32	Mon__2	9.3799	28.9318
2.7848	90.000	91.298	90.000	113.717	11.947	1290.134	.000	17.353		
.000 rb72 = (No title provided yet)										
20	48.09	1567.506	2.03	A	LOSHv6.1a	20Mar01	17:11:56	217	9.3820	57.8616
2.8888	90.000	91.696	90.000	113.7081	2.9869	1199.3670	.0000	21.8599		
.0000 rb72 = (No title provided yet)										
20	47.69	905.490	1.17	P	LOSHv6.1a	20Mar01	17:11:56	38	9.4280	28.9288
3.3376	90.000	95.895	90.000	113.7027	11.9492	907.2547	.0000	65.9762		
.0000 rb72 = (No title provided yet)										
20	47.42	779.003	1.01	P	LOSHv6.1a	20Mar01	17:11:56	8	9.4450	28.9308
2.8713	90.000	96.837	90.000	113.7079	11.9476	1230.4060	.0000	89.0502		
.0000 rb72 = (No title provided yet)										
20	47.11	1562.581	2.02	A	LOSHv6.1a	20Mar01	17:11:56	220	9.4146	57.8619
2.8797	90.000	95.065	90.000	113.7082	2.9869	1215.3680	.0000	65.6452		
.0000 rb72 = (No title provided yet)										
20	47.0	767.095	.99	P	DICVOL91/log	20Mar01	16:51:32	Mon__9	9.3928	28.9322
2.8273	90.000	93.250	90.000	113.712	11.946	1255.031	.000	42.834		
.000 rb72 = (No title provided yet)										
20	46.97	785.276	1.02	P	LOSHv6.1a	20Mar01	17:11:56	290	9.3807	28.9308
2.8944	90.000	91.397	90.000	113.7080	11.9476	1194.3810	.0000	17.9696		
.0000 rb72 = (No title provided yet)										
20	46.9	752.151	.97	P	DICVOL91/log	20Mar01	16:51:32	Mon_15	28.9390	9.3774
2.7724	90.000	91.330	90.000	11.947	113.720	1301.734	.000	5.789		
.000 rb72 = (No title provided yet)										
20	46.9	752.151	.97	P	DICVOL91/log	20Mar01	16:51:32	Mon_13	28.9390	9.3774
2.7724	90.000	91.330	90.000	11.947	113.720	1301.734	.000	5.789		
.000 rb72 = (No title provided yet)										
20	46.7	752.188	.97	P	DICVOL91/log	20Mar01	16:51:32	Mon_24	29.0076	9.3778
2.7724	90.000	94.154	90.000	11.947	113.710	1307.896	.000	18.110		
.000 rb72 = (No title provided yet)										
20	46.7	752.188	.97	P	DICVOL91/log	20Mar01	16:51:32	Mon_19	29.0076	9.3778
2.7724	90.000	94.154	90.000	11.947	113.710	1307.896	.000	18.110		
.000 rb72 = (No title provided yet)										
20	46.38	818.355	1.06	P	LOSHv6.1a	20Mar01	17:11:56	23	9.3806	28.9307
3.0163	90.000	91.371	90.000	113.7066	11.9476	1099.7600	.0000	16.9269		
.0000 rb72 = (No title provided yet)										
20	45.76	978.221	1.26	P	LOSHv6.1a	20Mar01	17:11:56	473	9.4166	28.9299
3.6056	90.000	95.190	90.000	113.7048	11.9483	775.5493	.0000	53.7288		
.0000 rb72 = (No title provided yet)										
20	45.30	1639.109	2.12	A	LOSHv6.1a	20Mar01	17:11:56	235	9.3782	57.8620
3.0207	90.000	90.480	90.000	113.7079	2.9868	1096.0020	.0000	5.9197		
.0000 rb72 = (No title provided yet)										
20	45.03	776.001	1.00	P	LOSHv6.1a	20Mar01	17:11:56	73	28.9536	9.3778
2.8603	90.000	92.287	90.000	11.9478	113.7101	1224.2830	.0000	9.6509		
.0000 rb72 = (No title provided yet)										
20	44.8	744.393	.96	P	DICVOL91/log	20Mar01	16:51:32	Mon_27	9.4105	28.9336
2.7435	90.000	94.787	90.000	113.713	11.945	1337.905	.000	65.100		
.000 rb72 = (No title provided yet)										

20	44.7	742.775	.96	P	DICVOL91/log	20Mar01	16:51:32	Mon_22	28.9740	9.3770
2.7380	90.000	93.131	90.000	11.948	113.729	1337.922	.000	13.811		
.000 rb72 = (No title provided yet)										
20	44.7	742.775	.96	P	DICVOL91/log	20Mar01	16:51:32	Mon_17	28.9740	9.3770
2.7380	90.000	93.131	90.000	11.948	113.729	1337.922	.000	13.811		
.000 rb72 = (No title provided yet)										
20	44.16	773.876	1.00	P	LOSHv6.1a	20Mar01	17:11:56	2	9.3826	28.9317
2.8523	90.000	91.817	90.000	113.7079	11.9468	1230.4130	.0000	23.7219		
.0000 rb72 = (No title provided yet)										
20	43.91	1706.480	2.21	A	LOSHv6.1a	20Mar01	17:11:56	386	9.3875	57.8617
3.1449	90.000	92.597	90.000	113.7083	2.9869	1013.1670	.0000	30.7588		
.0000 rb72 = (No title provided yet)										
20	43.0	748.471	.97	P	DICVOL91/log	20Mar01	16:51:32	Mon_21	28.9544	9.3770
2.7590	90.000	92.316	90.000	11.948	113.729	1315.850	.000	10.134		
.000 rb72 = (No title provided yet)										
20	43.0	748.471	.97	P	DICVOL91/log	20Mar01	16:51:32	Mon_16	28.9544	9.3770
2.7590	90.000	92.316	90.000	11.948	113.729	1315.850	.000	10.134		
.000 rb72 = (No title provided yet)										
20	42.9	766.510	.99	P	DICVOL91/log	20Mar01	16:51:32	Mon_5	9.3856	28.9335
2.8250	90.000	92.345	90.000	113.711	11.945	1255.136	.000	30.915		
.000 rb72 = (No title provided yet)										
20	42.67	782.357	1.01	P	LOSHv6.1a	20Mar01	17:11:56	216	28.9493	9.3779
2.8836	90.000	92.032	90.000	11.9473	113.7078	1204.1350	.0000	8.5046		
.0000 rb72 = (No title provided yet)										
20	42.5	756.773	.98	P	DICVOL91/log	20Mar01	16:51:32	Mon_14	28.9322	9.3770
2.7896	90.000	90.574	90.000	11.948	113.729	1285.168	.000	2.483		
.000 rb72 = (No title provided yet)										
20	42.5	756.773	.98	P	DICVOL91/log	20Mar01	16:51:32	Mon_12	28.9322	9.3770
2.7896	90.000	90.574	90.000	11.948	113.729	1285.168	.000	2.483		
.000 rb72 = (No title provided yet)										
20	42.36	807.491	1.04	P	LOSHv6.1a	20Mar01	17:11:56	20	9.3791	28.9304
2.9763	90.000	90.962	90.000	113.7103	11.9479	1129.1610	.0000	12.0359		
.0000 rb72 = (No title provided yet)										
20	42.31	1911.244	2.47	A	LOSHv6.1a	20Mar01	17:11:56	401	9.4110	57.8606
3.5223	90.000	94.810	90.000	113.7074	2.9870	811.7256	.0000	50.9463		
.0000 rb72 = (No title provided yet)										
20	42.20	775.665	1.00	P	LOSHv6.1a	20Mar01	17:11:56	75	28.9374	9.3779
2.8590	90.000	91.229	90.000	11.9476	113.7073	1224.0040	.0000	5.1863		
.0000 rb72 = (No title provided yet)										
20	42.14	863.699	1.12	P	LOSHv6.1a	20Mar01	17:11:56	32	9.4934	28.9308
3.1834	90.000	98.949	90.000	113.7079	11.9476	1011.2100	.0000	105.4889		
.0000 rb72 = (No title provided yet)										
20	41.96	779.539	1.01	P	LOSHv6.1a	20Mar01	17:11:56	143	28.9407	9.3777
2.8732	90.000	91.468	90.000	11.9472	113.7113	1212.1060	.0000	6.1676		
.0000 rb72 = (No title provided yet)										
20	41.79	779.543	1.01	P	LOSHv6.1a	20Mar01	17:11:56	214	28.9407	9.3777
2.8733	90.000	91.470	90.000	11.9472	113.7112	1212.0910	.0000	6.1731		
.0000 rb72 = (No title provided yet)										
20	41.41	789.976	1.02	P	LOSHv6.1a	20Mar01	17:11:56	289	28.9312	9.3779
2.9117	90.000	90.349	90.000	11.9477	113.7072	1179.5520	.0000	1.4449		
.0000 rb72 = (No title provided yet)										
20	41.37	815.925	1.05	P	LOSHv6.1a	20Mar01	17:11:56	444	9.4659	28.9306
3.0074	90.000	97.820	90.000	113.7087	11.9477	1126.5110	.0000	97.3895		
.0000 rb72 = (No title provided yet)										
20	41.3	775.597	1.00	P	DICVOL91/log	20Mar01	16:51:32	Mon_20	29.0190	9.3777
2.8587	90.000	94.450	90.000	11.947	113.712	1231.077	.000	18.819		
.000 rb72 = (No title provided yet)										
20	40.99	846.017	1.09	P	LOSHv6.1a	20Mar01	17:11:56	29	9.4290	28.9320
3.1182	90.000	95.972	90.000	113.7093	11.9466	1039.7490	.0000	71.5433		
.0000 rb72 = (No title provided yet)										
20	40.65	828.521	1.07	P	LOSHv6.1a	20Mar01	17:11:56	447	9.4978	28.9311
3.0538	90.000	99.123	90.000	113.7120	11.9473	1099.9530	.0000	112.1440		
.0000 rb72 = (No title provided yet)										

20	39.70	789.216	1.02	P	LOSHv6.1a	20Mar01	17:11:56	14	9.4311	28.9309
2.9089	90.000	96.094	90.000	113.7099	11.9474	1195.2440	.0000	78.2712		
.0000 rb72 = (No title provided yet)										
20	39.6	748.103	.97	P	DICVOL91/log	20Mar01	16:51:32	Mon_23	28.9864	9.3773
2.7572	90.000	93.431	90.000	11.945	113.722	1320.145	.000	15.030		
.000 rb72 = (No title provided yet)										
20	39.6	748.103	.97	P	DICVOL91/log	20Mar01	16:51:32	Mon_18	28.9864	9.3773
2.7572	90.000	93.431	90.000	11.945	113.722	1320.145	.000	15.030		
.000 rb72 = (No title provided yet)										
20	39.59	1645.671	2.13	A	LOSHv6.1a	20Mar01	17:11:56	377	9.4182	57.8630
3.0328	90.000	95.304	90.000	113.7079	2.9867	1096.6110	.0000	65.2861		
.0000 rb72 = (No title provided yet)										
20	39.54	776.184	1.00	P	LOSHv6.1a	20Mar01	17:11:56	141	28.9324	9.3778
2.8609	90.000	90.692	90.000	11.9480	113.7090	1221.9230	.0000	2.9196		
.0000 rb72 = (No title provided yet)										
20	38.82	2054.889	2.66	A	LOSHv6.1a	20Mar01	17:11:56	262	9.3844	57.8613
3.7870	90.000	92.140	90.000	113.7083	2.9869	698.2535	.0000	21.0435		
.0000 rb72 = (No title provided yet)										
20	38.78	776.136	1.00	P	LOSHv6.1a	20Mar01	17:11:56	5	9.4009	28.9307
2.8607	90.000	94.012	90.000	113.7078	11.9477	1227.9570	.0000	52.2932		
.0000 rb72 = (No title provided yet)										
20	38.44	2105.177	2.72	A	LOSHv6.1a	20Mar01	17:11:56	408	9.3886	57.8615
3.8797	90.000	92.734	90.000	113.7073	2.9869	665.8898	.0000	26.2458		
.0000 rb72 = (No title provided yet)										
20	38.14	894.089	1.16	P	LOSHv6.1a	20Mar01	17:11:56	248	9.4742	28.9450
3.2956	91.868	98.173	89.734	113.7055	11.9486	940.7209	6.8425	92.9371		
.0000 rb72 = (No title provided yet)										
20	38.05	937.969	1.21	P	LOSHv6.1a	20Mar01	17:11:56	41	9.3902	28.9307
3.4573	90.000	92.950	90.000	113.7120	11.9476	838.8574	.0000	31.7919		
.0000 rb72 = (No title provided yet)										
20	37.97	961.867	1.24	P	LOSHv6.1a	20Mar01	17:11:56	44	9.3794	28.9277
3.5456	90.000	90.983	90.000	113.7047	11.9502	795.6943	.0000	10.3225		
.0000 rb72 = (No title provided yet)										
20	36.93	958.944	1.24	P	LOSHv6.1a	20Mar01	17:11:56	256	9.3884	28.9680
3.5347	92.971	92.697	89.860	113.7061	11.9490	804.3137	10.1519	28.4196		
.0000 rb72 = (No title provided yet)										
20	36.71	809.989	1.05	P	LOSHv6.1a	20Mar01	17:11:56	160	9.3801	28.9342
2.9855	90.812	91.274	89.982	113.7107	11.9472	1122.7340	3.2807	15.8840		
.0000 rb72 = (No title provided yet)										
20	36.68	2148.928	2.78	A	LOSHv6.1a	20Mar01	17:11:56	123	9.4401	57.8605
3.9603	90.000	96.579	90.000	113.7056	2.9870	646.0666	.0000	62.1067		
.0000 rb72 = (No title provided yet)										
20	35.49	1038.240	1.34	P	LOSHv6.1a	20Mar01	17:11:56	50	9.4075	28.9305
3.8268	90.000	94.538	90.000	113.7055	11.9478	687.1646	.0000	44.2305		
.0000 rb72 = (No title provided yet)										
20	35.02	1176.243	1.52	P	LOSHv6.1a	20Mar01	17:11:56	59	9.6040	28.9303
4.3356	90.000	102.464	90.000	113.7129	11.9480	557.9813	.0000	108.7328		
.0000 rb72 = (No title provided yet)										
20	34.60	902.240	1.17	P	LOSHv6.1a	20Mar01	17:11:56	322	9.5020	28.9312
3.3255	90.000	99.272	90.000	113.7080	11.9472	928.3723	.0000	104.7026		
.0000 rb72 = (No title provided yet)										
20	34.53	2441.546	3.16	A	LOSHv6.1a	20Mar01	17:11:56	274	28.9717	18.7558
4.4996	90.000	93.044	90.000	11.9476	28.4269	495.3228	.0000	8.1714		
.0000 rb72 = (No title provided yet)										
20	34.41	794.012	1.03	P	LOSHv6.1a	20Mar01	17:11:56	360	28.9359	9.3779
2.9266	90.000	91.094	90.000	11.9477	113.7077	1167.9660	.0000	4.5129		
.0000 rb72 = (No title provided yet)										
20	34.39	775.507	1.00	P	LOSHv6.1a	20Mar01	17:11:56	3	28.9445	9.3777
2.8584	90.000	91.738	90.000	11.9473	113.7113	1225.0570	.0000	7.3403		
.0000 rb72 = (No title provided yet)										
20	34.04	982.159	1.27	P	LOSHv6.1a	20Mar01	17:11:56	118	28.9414	9.3776
3.6201	90.000	91.535	90.000	11.9474	113.7138	763.5948	.0000	5.1165		
.0000 rb72 = (No title provided yet)										

20	33.43	1139.579	1.47	P	LOSHv6.1a	20Mar01	17:11:56	483	9.4313	28.9286
4.2005	90.000	96.087	90.000	113.7013	11.9493	573.2072	.0000	54.1396		
.0000 rb72 = (No title provided yet)										
20	33.30	894.676	1.16	P	LOSHv6.1a	20Mar01	17:11:56	463	9.4520	28.9342
3.2979	91.178	97.173	89.853	113.7051	11.9498	934.3998	4.3116	81.3864		
.0000 rb72 = (No title provided yet)										
20	33.29	907.793	1.17	P	LOSHv6.1a	20Mar01	17:11:56	323	9.4505	28.9305
3.3460	90.000	97.104	90.000	113.7067	11.9478	907.0791	.0000	79.4350		
.0000 rb72 = (No title provided yet)										
20	33.20	985.195	1.27	P	LOSHv6.1a	20Mar01	17:11:56	188	28.9440	9.3778
3.6314	90.000	91.777	90.000	11.9481	113.7089	759.0663	.0000	5.9078		
.0000 rb72 = (No title provided yet)										
20	32.85	824.792	1.07	P	LOSHv6.1a	20Mar01	17:11:56	378	9.3916	28.9571
3.0400	92.414	93.107	89.869	113.7100	11.9471	1087.1700	9.5865	38.0793		
.0000 rb72 = (No title provided yet)										
20	32.54	1080.972	1.40	P	LOSHv6.1a	20Mar01	17:11:56	193	9.4439	28.9344
3.9844	91.036	96.772	89.878	113.7045	11.9485	639.0020	3.1364	63.5613		
.0000 rb72 = (No title provided yet)										
20	32.35	1234.632	1.60	P	LOSHv6.1a	20Mar01	17:11:56	62	9.5857	28.9307
4.5506	90.000	101.951	90.000	113.7070	11.9476	504.5350	.0000	99.1992		
.0000 rb72 = (No title provided yet)										
20	32.28	889.560	1.15	P	LOSHv6.1a	20Mar01	17:11:56	249	9.5085	28.9529
3.2788	92.274	99.500	89.625	113.7020	11.9482	957.7252	8.3729	108.8453		
.0000 rb72 = (No title provided yet)										
20	32.10	880.303	1.14	P	LOSHv6.1a	20Mar01	17:11:56	390	9.4497	28.9609
3.2446	92.622	97.062	89.678	113.7050	11.9478	966.4522	9.7567	81.4297		
.0000 rb72 = (No title provided yet)										
20	32.08	1194.670	1.54	P	LOSHv6.1a	20Mar01	17:11:56	486	9.4902	28.9299
4.4034	90.000	98.816	90.000	113.7027	11.9483	528.1404	.0000	75.1147		
.0000 rb72 = (No title provided yet)										
20	31.86	982.729	1.27	P	LOSHv6.1a	20Mar01	17:11:56	48	28.9561	9.3786
3.6224	90.640	92.494	89.972	11.9493	113.7052	763.6374	6.5796	8.3123		
.0000 rb72 = (No title provided yet)										
20	31.83	972.539	1.26	P	LOSHv6.1a	20Mar01	17:11:56	329	9.3878	28.9314
3.5846	90.000	92.646	90.000	113.7109	11.9471	779.9185	.0000	27.4934		
.0000 rb72 = (No title provided yet)										
20	31.75	919.184	1.19	P	LOSHv6.1a	20Mar01	17:11:56	251	9.4265	28.9482
3.3881	92.091	95.809	89.788	113.7028	11.9491	881.3177	7.4487	64.0330		
.0000 rb72 = (No title provided yet)										
20	31.57	934.958	1.21	P	LOSHv6.1a	20Mar01	17:11:56	324	9.4126	28.9379
3.4462	91.346	94.916	89.885	113.7046	11.9483	848.7310	4.7153	53.2239		
.0000 rb72 = (No title provided yet)										
20	31.31	3634.249	4.70	I	LOSHv6.1a	20Mar01	17:11:56	395	18.7561	57.8613
3.3488	90.000	90.000	90.000	28.4259	2.9869	891.7290	.0000	.0000		
.0000 rb72 = (No title provided yet)										
20	31.27	826.467	1.07	P	LOSHv6.1a	20Mar01	17:11:56	236	9.3802	28.9480
3.0462	91.937	91.289	89.956	113.7094	11.9470	1079.4640	7.6743	15.7492		
.0000 rb72 = (No title provided yet)										
20	31.18	798.935	1.03	P	LOSHv6.1a	20Mar01	17:11:56	366	9.4090	28.9589
2.9446	92.472	94.667	89.799	113.7093	11.9466	1163.1170	10.1343	59.1240		
.0000 rb72 = (No title provided yet)										
20	30.91	881.201	1.14	P	LOSHv6.1a	20Mar01	17:11:56	319	9.4683	28.9315
3.2481	90.736	97.916	89.899	113.7032	11.9490	966.3497	2.7340	91.2952		
.0000 rb72 = (No title provided yet)										
20	30.91	834.584	1.08	P	LOSHv6.1a	20Mar01	17:11:56	239	9.3928	28.9409
3.0760	91.413	93.236	89.920	113.7096	11.9465	1060.8940	5.5432	39.1970		
.0000 rb72 = (No title provided yet)										
20	30.77	2411.220	3.12	A	LOSHv6.1a	20Mar01	17:11:56	201	28.9437	18.7555
4.4436	90.000	91.640	90.000	11.9467	28.4279	506.8607	.0000	4.4528		
.0000 rb72 = (No title provided yet)										
20	30.6	775.533	1.00	P	DICVOL91/log	20Mar01	16:51:32	Mon_25	29.0325	9.3777
2.8584	90.000	94.765	90.000	11.946	113.712	1232.427	.000	20.159		
.000 rb72 = (No title provided yet)										

20	30.33	817.829	1.06	P	LOSHv6.1a	20Mar01	17:11:56	164	28.9408	9.3780
3.0143	90.167	91.451	89.996	11.9470	113.7065	1101.3220	2.0603	5.8075		
.0000 rb72 = (No title provided yet)										
20	30.31	781.155	1.01	P	LOSHv6.1a	20Mar01	17:11:56	82	9.4574	28.9360
2.8792	91.105	97.436	89.857	113.7094	11.9477	1227.2690	4.6317	96.6785		
.0000 rb72 = (No title provided yet)										
20	29.93	2216.291	2.87	A	LOSHv6.1a	20Mar01	17:11:56	413	9.4249	57.8537
4.0848	90.000	95.698	90.000	113.6975	2.9877	605.2859	.0000	52.0901		
.0000 rb72 = (No title provided yet)										
20	29.91	795.012	1.03	P	LOSHv6.1a	20Mar01	17:11:56	226	9.4698	28.9624
2.9302	92.627	97.993	89.635	113.7091	11.9466	1190.1110	10.8257	102.1987		
.0000 rb72 = (No title provided yet)										
20	29.88	802.688	1.04	P	LOSHv6.1a	20Mar01	17:11:56	369	9.4531	28.9559
2.9585	92.352	97.233	89.704	113.7093	11.9470	1162.8170	9.5969	91.4916		
.0000 rb72 = (No title provided yet)										
20	29.62	805.352	1.04	P	LOSHv6.1a	20Mar01	17:11:56	230	9.4022	28.9525
2.9682	92.096	94.137	89.849	113.7112	11.9456	1142.5110	8.5221	51.9756		
.0000 rb72 = (No title provided yet)										

I20	Merit	Volume	V/V1	BL	IndexProg	Date	Time	Pedig	a	b
c	alpha	beta	gamma	Q(A)	Q(B)	Q(C)	Q(D)	Q(E)		
Q(F)	Description (up to 80-chars, from Run-Title line)									
20	52.3	981.918	1.00	P	DICVOL91/log	20Mar01	17:24:58	Mon_15	28.9433	9.3779
3.6194	90.000	91.803	90.000	11.949	113.707	764.112	.000	6.013		
.000 rb73 = (No title provided yet)										
20	45.2	984.864	1.00	P	DICVOL91/log	20Mar01	17:24:58	Mon_27	9.4648	28.9267
3.6307	90.000	97.788	90.000	113.717	11.951	772.802	.000	80.342		
.000 rb73 = (No title provided yet)										
20	45.1	984.878	1.00	P	DICVOL91/log	20Mar01	17:24:58	Mon_20	9.4648	28.9279
3.6306	90.000	97.788	90.000	113.717	11.950	772.844	.000	80.344		
.000 rb73 = (No title provided yet)										
20	45.1	984.878	1.00	P	DICVOL91/log	20Mar01	17:24:58	Mon_19	9.4648	28.9279
3.6306	90.000	97.788	90.000	113.717	11.950	772.844	.000	80.344		
.000 rb73 = (No title provided yet)										
20	43.2	984.907	1.00	P	DICVOL91/log	20Mar01	17:24:58	Mon_28	9.4656	28.9263
3.6306	90.000	97.788	90.000	113.698	11.951	772.844	.000	80.337		
.000 rb73 = (No title provided yet)										
20	37.42	1984.831	2.02	A	LOSHv6.1a	20Mar01	17:40:08	35	9.5368	57.8779
3.6571	90.000	100.499	90.000	113.7270	2.9852	773.3570	.0000	108.0797		
.0000 rb73 = (No title provided yet)										
20	33.6	962.890	.98	P	DICVOL91/log	20Mar01	17:24:58	Mon_26	9.4520	28.9377
3.5482	90.000	97.180	90.000	113.708	11.942	806.904	.000	75.718		
.000 rb73 = (No title provided yet)										
20	33.41	1019.581	1.04	P	LOSHv6.1a	20Mar01	17:40:08	105	9.5094	28.9393
3.7573	90.000	99.575	90.000	113.7312	11.9405	728.5173	.0000	95.7631		
.0000 rb73 = (No title provided yet)										
20	32.8	938.439	.96	P	DICVOL91/log	20Mar01	17:24:58	Mon_11	28.9400	9.3781
3.4588	90.000	91.417	90.000	11.947	113.703	836.401	.000	4.944		
.000 rb73 = (No title provided yet)										
20	32.0	935.943	.95	P	DICVOL91/log	20Mar01	17:24:58	Mon_10	28.9315	9.3781
3.4500	90.000	90.915	90.000	11.950	113.703	840.374	.000	3.201		
.000 rb73 = (No title provided yet)										
20	31.93	1166.402	1.19	P	LOSHv6.1a	20Mar01	17:40:08	457	9.5954	28.9374
4.2985	90.000	102.240	90.000	113.7223	11.9421	566.6918	.0000	107.6367		
.0000 rb73 = (No title provided yet)										
20	31.88	2119.794	2.16	A	LOSHv6.1a	20Mar01	17:40:08	38	9.3784	57.8779
3.9059	90.000	91.062	90.000	113.7338	2.9852	655.6898	.0000	10.1238		
.0000 rb73 = (No title provided yet)										
20	31.78	1094.872	1.12	P	LOSHv6.1a	20Mar01	17:40:08	192	28.9559	9.3769
4.0349	90.000	92.011	90.000	11.9416	113.7311	614.9897	.0000	6.0151		
.0000 rb73 = (No title provided yet)										

20	30.78	1271.865	1.30 P	LOSHv6.1a	20Mar01	17:40:08	79	9.5617	28.9440
4.6864	90.000	101.294	90.000	113.7413	11.9367	473.4802	.0000	90.8975	
.0000 rb73 = (No title provided yet)									
20	30.78	1271.864	1.30 P	LOSHv6.1a	20Mar01	17:40:08	323	9.5617	28.9440
4.6864	90.000	101.294	90.000	113.7412	11.9367	473.4803	.0000	90.8974	
.0000 rb73 = (No title provided yet)									
20	30.66	1161.283	1.18 P	LOSHv6.1a	20Mar01	17:40:08	500	9.6058	28.9375
4.2796	90.000	102.525	90.000	113.7245	11.9420	572.9479	.0000	110.7185	
.0000 rb73 = (No title provided yet)									
20	29.18	1160.572	1.18 P	LOSHv6.1a	20Mar01	17:40:08	75	9.5013	28.9465
4.2775	91.681	99.272	89.729	113.7259	11.9448	561.5687	4.7421	81.3996	
.0000 rb73 = (No title provided yet)									
20	28.8	937.104	.95 P	DICVOL91/log	20Mar01	17:24:58 Mon_24	9.4563	28.9366	
3.4536	90.000	97.421	90.000	113.727	11.943	852.633	.000	80.439	
.000 rb73 = (No title provided yet)									
20	28.52	2097.248	2.14 A	LOSHv6.1a	20Mar01	17:40:08	151	9.4327	57.8727
3.8644	90.000	96.190	90.000	113.7134	2.9857	677.5112	.0000	59.8588	
.0000 rb73 = (No title provided yet)									
20	28.33	1525.955	1.55 P	LOSHv6.1a	20Mar01	17:40:08	246	9.4276	28.9395
5.6233	90.000	95.944	90.000	113.7320	11.9404	319.6675	.0000	39.4942	
.0000 rb73 = (No title provided yet)									
20	28.31	2018.349	2.06 A	LOSHv6.1a	20Mar01	17:40:08	147	9.4436	57.8819
3.7188	90.000	96.823	90.000	113.7370	2.9848	733.4372	.0000	68.6213	
.0000 rb73 = (No title provided yet)									
20	28.3	936.461	.95 P	DICVOL91/log	20Mar01	17:24:58 Mon__4	9.3800	28.9310	
3.4517	90.000	91.286	90.000	113.714	11.947	839.755	.000	13.871	
.000 rb73 = (No title provided yet)									
20	28.3	936.461	.95 P	DICVOL91/log	20Mar01	17:24:58 Mon__1	9.3800	28.9310	
3.4517	90.000	91.286	90.000	113.714	11.947	839.755	.000	13.871	
.000 rb73 = (No title provided yet)									
20	28.00	1135.091	1.16 P	LOSHv6.1a	20Mar01	17:40:08	456	9.5881	28.9662
4.1835	92.634	102.046	89.450	113.7305	11.9436	598.6133	7.6020	108.7982	
.0000 rb73 = (No title provided yet)									
20	27.56	996.015	1.01 P	LOSHv6.1a	20Mar01	17:40:08	103	9.3983	28.9631
3.6705	92.323	93.878	89.843	113.7355	11.9405	746.8801	7.6394	39.3956	
.0000 rb73 = (No title provided yet)									
20	27.5	935.184	.95 P	DICVOL91/log	20Mar01	17:24:58 Mon_23	9.4478	28.9416	
3.4459	90.000	97.010	90.000	113.725	11.939	854.893	.000	76.107	
.000 rb73 = (No title provided yet)									
20	27.12	994.738	1.01 P	LOSHv6.1a	20Mar01	17:40:08	66	9.4518	28.9448
3.6659	91.438	97.185	89.820	113.7144	11.9435	756.4028	4.7326	73.3405	
.0000 rb73 = (No title provided yet)									
20	26.61	1024.727	1.04 P	LOSHv6.1a	20Mar01	17:40:08	223	9.3901	28.9523
3.7765	91.832	93.049	89.903	113.7338	11.9420	703.8669	5.8521	30.0863	
.0000 rb73 = (No title provided yet)									
20	26.52	1004.509	1.02 P	LOSHv6.1a	20Mar01	17:40:08	145	9.3851	28.9645
3.7018	92.344	92.455	89.900	113.7405	11.9397	732.3279	7.6405	24.7051	
.0000 rb73 = (No title provided yet)									
20	26.36	2313.545	2.36 A	LOSHv6.1a	20Mar01	17:40:08	412	9.4439	57.8723
4.2629	90.000	96.783	90.000	113.7108	2.9858	558.0664	.0000	59.5094	
.0000 rb73 = (No title provided yet)									
20	26.2	998.367	1.02 P	DICVOL91/log	20Mar01	17:24:58 Mon_14	28.9336	9.3779	
3.6797	90.000	90.674	90.000	11.947	113.707	738.644	.000	2.210	
.000 rb73 = (No title provided yet)									
20	26.15	1147.540	1.17 P	LOSHv6.1a	20Mar01	17:40:08	361	9.3926	28.9451
4.2291	91.434	93.263	89.918	113.7215	11.9432	561.2813	4.0907	28.7552	
.0000 rb73 = (No title provided yet)									
20	26.15	1147.540	1.17 P	LOSHv6.1a	20Mar01	17:40:08	232	9.3926	28.9451
4.2291	91.434	93.263	89.918	113.7215	11.9432	561.2816	4.0906	28.7553	
.0000 rb73 = (No title provided yet)									
20	25.97	1002.322	1.02 P	LOSHv6.1a	20Mar01	17:40:08	143	9.3818	28.9761
3.6939	93.038	91.704	89.910	113.7130	11.9438	735.5934	9.9299	17.1796	
.0000 rb73 = (No title provided yet)									

20	25.94	1655.432	1.69	P	LOSHv6.1a	20Mar01	17:40:08	132	9.3825	28.9370
6.1005	90.000	91.837	90.000	113.7138	11.9424	268.9792	.0000	11.2146		
.0000 rb73 = (No title provided yet)										
20	25.94	1655.432	1.69	P	LOSHv6.1a	20Mar01	17:40:08	91	9.3825	28.9370
6.1005	90.000	91.837	90.000	113.7138	11.9424	268.9792	.0000	11.2146		
.0000 rb73 = (No title provided yet)										
20	25.86	1345.237	1.37	P	LOSHv6.1a	20Mar01	17:40:08	371	9.6475	28.9409
4.9587	91.555	103.594	89.635	113.7235	11.9480	430.7653	3.7840	104.0100		
.0000 rb73 = (No title provided yet)										
20	25.6	947.094	.96	P	DICVOL91/log	20Mar01	17:24:58	Mon_21	9.4873	28.9302
3.4908	90.000	98.700	90.000	113.702	11.948	839.851	.000	93.485		
.000 rb73 = (No title provided yet)										
20	25.32	1080.476	1.10	P	LOSHv6.1a	20Mar01	17:40:08	356	9.4849	28.9442
3.9820	91.235	98.660	89.814	113.7339	11.9421	645.5894	3.7416	81.5800		
.0000 rb73 = (No title provided yet)										
20	25.01	1064.789	1.08	P	LOSHv6.1a	20Mar01	17:40:08	310	9.4015	28.9408
3.9237	90.000	94.140	90.000	113.7308	11.9393	652.9606	.0000	39.3498		
.0000 rb73 = (No title provided yet)										
20	24.97	1056.146	1.08	P	LOSHv6.1a	20Mar01	17:40:08	152	9.4046	28.9669
3.8919	92.467	94.395	89.811	113.7298	11.9399	665.3247	7.6506	42.1163		
.0000 rb73 = (No title provided yet)										
20	24.89	991.723	1.01	P	LOSHv6.1a	20Mar01	17:40:08	102	9.4078	28.9360
3.6550	90.707	94.576	89.944	113.7099	11.9451	753.4799	2.3343	46.6995		
.0000 rb73 = (No title provided yet)										
20	24.75	1009.042	1.03	P	LOSHv6.1a	20Mar01	17:40:08	148	9.4298	28.9506
3.7182	91.469	96.073	89.845	113.7324	11.9391	731.9792	4.7651	61.0334		
.0000 rb73 = (No title provided yet)										
20	24.7	947.246	.96	P	DICVOL91/log	20Mar01	17:24:58	Mon_29	9.4879	28.9331
3.4908	90.000	98.701	90.000	113.688	11.946	839.855	.000	93.490		
.000 rb73 = (No title provided yet)										
20	24.69	1009.042	1.03	P	LOSHv6.1a	20Mar01	17:40:08	186	9.4298	28.9506
3.7182	91.469	96.073	89.845	113.7324	11.9390	731.9805	4.7649	61.0343		
.0000 rb73 = (No title provided yet)										
20	24.32	1086.350	1.11	P	LOSHv6.1a	20Mar01	17:40:08	156	28.9764	9.3774
4.0037	90.110	93.066	89.994	11.9442	113.7191	625.6293	1.0201	9.2468		
.0000 rb73 = (No title provided yet)										
20	24.3	934.510	.95	P	DICVOL91/log	20Mar01	17:24:58	Mon__9	28.9418	9.3769
3.4440	90.000	90.982	90.000	11.942	113.732	843.337	.000	3.440		
.000 rb73 = (No title provided yet)										
20	24.16	1027.772	1.05	P	LOSHv6.1a	20Mar01	17:40:08	150	9.4785	28.9885
3.7874	93.270	98.417	89.522	113.7439	11.9389	714.6710	10.4252	83.3365		
.0000 rb73 = (No title provided yet)										
20	24.15	1043.840	1.06	P	LOSHv6.1a	20Mar01	17:40:08	267	9.3892	28.9666
3.8466	92.440	92.956	89.874	113.7368	11.9397	678.8627	7.6545	28.6359		
.0000 rb73 = (No title provided yet)										
20	24.13	1192.733	1.21	P	LOSHv6.1a	20Mar01	17:40:08	233	9.4679	28.9428
4.3959	91.382	97.930	89.809	113.7215	11.9446	527.8290	3.7944	67.5844		
.0000 rb73 = (No title provided yet)										
20	23.65	1010.586	1.03	P	LOSHv6.1a	20Mar01	17:40:08	183	9.3791	28.9602
3.7244	92.259	91.311	89.948	113.7367	11.9419	722.4073	7.3219	13.1036		
.0000 rb73 = (No title provided yet)										
20	23.41	1076.163	1.10	P	LOSHv6.1a	20Mar01	17:40:08	270	9.4989	28.9627
3.9664	92.601	99.164	89.586	113.7130	11.9458	653.5032	7.9166	86.7448		
.0000 rb73 = (No title provided yet)										
20	23.38	1053.418	1.07	P	LOSHv6.1a	20Mar01	17:40:08	227	9.4952	28.9498
3.8818	91.454	99.057	89.771	113.7327	11.9396	680.9172	4.5189	87.5866		
.0000 rb73 = (No title provided yet)										
20	23.38	1018.661	1.04	P	LOSHv6.1a	20Mar01	17:40:08	36	9.4584	28.9627
3.7541	92.356	97.536	89.691	113.7355	11.9414	723.1773	7.5744	75.1609		
.0000 rb73 = (No title provided yet)										
20	23.18	1043.118	1.06	P	LOSHv6.1a	20Mar01	17:40:08	9	9.3893	28.9699
3.8438	92.561	92.940	89.869	113.7306	11.9392	679.9715	8.0426	28.4945		
.0000 rb73 = (No title provided yet)										

20	23.18	998.457	1.02	P	LOSHv6.1a	20Mar01	17:40:08	104	9.4297	28.9460
3.6791	90.970	96.063	89.898	113.7315	11.9385	747.3232		3.1810	61.5814	
.0000 rb73 = (No title provided yet)										
20	23.17	1640.279	1.67	P	LOSHv6.1a	20Mar01	17:40:08	335	9.4289	28.9404
6.0444	90.000	96.022	90.000	113.7317	11.9396	276.7581		.0000	37.2269	
.0000 rb73 = (No title provided yet)										
20	23.17	1003.183	1.02	P	LOSHv6.1a	20Mar01	17:40:08	185	9.3952	28.9430
3.6970	91.144	93.545	89.929	113.7246	11.9423	734.7428		3.7345	35.7423	
.0000 rb73 = (No title provided yet)										
20	22.98	987.298	1.01	P	LOSHv6.1a	20Mar01	17:40:08	65	9.3949	28.9482
3.6383	91.493	93.524	89.908	113.7253	11.9413	758.8114		4.9511	36.1044	
.0000 rb73 = (No title provided yet)										
20	22.96	1015.338	1.03	P	LOSHv6.1a	20Mar01	17:40:08	187	9.4704	28.9551
3.7413	91.757	98.056	89.754	113.7302	11.9387	729.3895		5.6644	80.6916	
.0000 rb73 = (No title provided yet)										
20	22.86	1750.642	1.78	P	LOSHv6.1a	20Mar01	17:40:08	94	9.4058	28.9304
6.4521	90.000	94.353	90.000	113.6889	11.9479	241.6044		.0000	25.1596	
.0000 rb73 = (No title provided yet)										
20	22.82	1307.986	1.33	P	LOSHv6.1a	20Mar01	17:40:08	81	9.5165	28.9374
4.8200	90.000	99.795	90.000	113.7110	11.9421	443.2666		.0000	76.3913	
.0000 rb73 = (No title provided yet)										

McMAILLE

With b and c fixed, searching for an orthorhombic cell. There could be a solution ?? 47 indexed reflections.

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FINAL LIST OF CELL PROPOSALS, sorted by Rp :
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Rp	Vol	Vol/V1	Ind	Nsol	a	b	c	alpha	beta	gamma
0.089	1029.523	1.00	47	28	3.7970	9.3682	28.9430	90.000	90.000	90.000
0.133	1070.535	1.04	47	60	3.9479	9.3706	28.9381	90.000	90.000	90.000