

SAMPLE 1:

Monoclinic a=10.318 b=7.393 c=8.527 Beta=91.3

SG: P2 (Best Cell CheckCell)

Crysfire used / CDT file without pics from cubic phase (found in the database ICDD PDF 2001)/ **DICVOL** gave the best solution

Cell was checked with **Checkcell and Winplotr-Fullprof** (whole pattern fitting, Le Bail Fit)

MONOCLINIC SYSTEM

DIRECT PARAMETERS : A=10.3240 B= 7.3963 C= 8.5337 BETA= 91.302

VOLUME= 651.47

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
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0	1	0	7.40001	7.39633	.00368	.01826	.01828	11.950	11.956	-.006
1	0	-1	6.65226	6.65048	.00177	.02260	.02261	13.299	13.303	-.004
1	0	1	6.50094	6.50368	-.00275	.02366	.02364	13.610	13.604	.006
2	0	0	5.16201	5.16068	.00134	.03753	.03755	17.164	17.168	-.004
1	1	-1	4.94728	4.94533	.00195	.04086	.04089	17.915	17.922	-.007
1	1	1	4.88402	4.88407	-.00005	.04192	.04192	18.149	18.149	.000
0	0	2	4.26531	4.26576	-.00045	.05497	.05496	20.809	20.807	.002
2	1	-1	3.82111	3.81985	.00126	.06849	.06853	23.260	23.268	-.008
2	1	1	3.76226	3.76359	-.00132	.07065	.07060	23.629	23.621	.008
0	1	2	3.69856	3.69523	.00333	.07310	.07323	24.042	24.064	-.022
0	2	0	3.69816	.00040	.07312	24.045	-.003			
1	1	-2	3.49961	3.50093	-.00131	.08165	.08159	25.431	25.421	.010
1	1	2	3.46068	3.45746	.00322	.08350	.08365	25.722	25.746	-.024
2	0	-2	3.32606	3.32524	.00082	.09039	.09044	26.782	26.789	-.007
1	2	-1	3.23138	3.23206	-.00068	.09577	.09573	27.582	27.576	.006
1	2	1	3.21538	3.21478	.00060	.09672	.09676	27.722	27.727	-.005
3	0	-1	3.21622	-.00084	.09667	27.715	.007			
3	0	1	3.16537	3.16592	-.00056	.09981	.09977	28.169	28.164	.005
2	1	-2	3.03254	3.03283	-.00029	.10874	.10872	29.430	29.427	.003
2	2	0	3.00588	3.00602	-.00014	.11068	.11067	29.697	29.696	.001
3	1	1	2.91048	2.91050	-.00002	.11805	.11805	30.694	30.694	.000
1	1	-3	2.58339	2.58400	-.00061	.14984	.14977	34.696	34.688	.008

* NUMBER OF LINES

.- INPUT DATA = 20

.- CALCULATED = 49

* FIGURES OF MERIT

1.- M(20) = 43.6

(REF. 4)

2.- F(20) = 69.1(.0059, 49)

(REF. 5)

SAMPLE 2:

Monoclinic a=19.880 b=8.195 c=11.242 Beta=106.06

SG: P21/N (Best Cell CheckCell)

Crysfire used / CDT / **DICVOL** gave the best solution

Cell was checked with **Checkcell and Winplotr-Fullprof** (whole pattern fitting, Le Bail Fit)

MONOCLINIC SYSTEM

DIRECT PARAMETERS : A=19.8661 B= 8.1965 C=11.2183 BETA=105.951

VOLUME=1756.38

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
0	0	1	10.76587	10.78643	-.02057	.00863	.00859	4.246	4.238	.008
2	0	0	9.55175	9.55061	.00114	.01096	.01096	4.786	4.787	-.001
1	0	1	8.45384	8.45053	.00332	.01399	.01400	5.408	5.410	-.002
1	1	0	7.53258	7.53230	.00029	.01762	.01763	6.070	6.070	.000
0	1	1	6.52539	6.52608	-.00070	.02348	.02348	7.008	7.007	.001
2	1	0	6.21961	6.21994	-.00033	.02585	.02585	7.353	7.353	.000
1	1	1	5.88402	5.88355	.00047	.02888	.02889	7.773	7.774	-.001
1	1	1	5.86593	5.88355	-.01762	.02906	.02889	7.797	7.774	.023
0	0	2	5.40123	5.39322	.00802	.03428	.03438	8.469	8.482	-.013
0	0	2	5.38347	5.39322	-.00975	.03450	.03438	8.497	8.482	.015
3	1	0	5.02797	5.02823	-.00027	.03956	.03955	9.099	9.099	.000
3	0	1	4.92217	4.92277	-.00060	.04127	.04126	9.295	9.294	.001
4	0	0	4.77557	4.77531	.00026	.04385	.04385	9.581	9.582	-.001
1	1	-2	4.63419	4.62892	.00527	.04656	.04667	9.874	9.885	-.011
0	1	2	4.49701	4.50539	-.00838	.04945	.04926	10.176	10.157	.019
2	0	2	4.22696	4.22526	.00169	.05597	.05601	10.828	10.832	-.004
4	0	-2	4.20104	4.19252	.00852	.05666	.05689	10.895	10.917	-.022
1	1	2	4.17886	4.17608	.00279	.05726	.05734	10.953	10.960	-.007
1	1	2	4.16144	4.17608	-.01464	.05774	.05734	10.999	10.960	.039
4	1	0	4.12591	4.12612	-.00021	.05874	.05874	11.094	11.093	.001
0	2	0	4.09756	4.09824	-.00068	.05956	.05954	11.171	11.169	.002
1	2	0	4.00641	4.00705	-.00064	.06230	.06228	11.426	11.424	.002
5	0	-1	3.96320	3.95975	.00345	.06367	.06378	11.551	11.561	-.010
0	2	1	3.83069	3.83104	-.00036	.06815	.06813	11.952	11.951	.001
2	2	0	3.76540	3.76615	-.00075	.07053	.07050	12.160	12.158	.002

* NUMBER OF LINES

.- INPUT DATA = 40

.- CALCULATED = 80

* FIGURES OF MERIT

1.- M(40) = 10.3

(REF. 4)

2.- F(40) = 87.8(.0057, 80)

(REF. 5)

SAMPLE 3:

Tetragonal a=13.3495 b=13.3495 c=9.4393

SG: P 42MM/C (Best Cell CheckCell)

Crysfire used / CDT / **TREOR** gave the best solution

Cell was checked with **Checkcell and Winplotr-Fullprof** (whole pattern fitting, Le Bail Fit)

A = 13.354580 .000914 A ALFA = 90.000000 .000000 DEG
B = 13.354580 .000914 A BETA = 90.000000 .000000 DEG
C = 9.442072 .000824 A GAMMA = 90.000000 .000000 DEG

UNIT CELL VOLUME = 1683.94 A**3

H	K	L	SST-OBS	SST-CALC	DELTA	2TH-OB	2TH-CA	D-OBS	FREE PARAM.
1	0	0	.000892	.000892	.000000	3.423	3.423	13.3549	1
0	0	1	.001784	.001784	.000000	4.841	4.842	9.4425	15
1	0	1	.002676	.002676	.000000	5.931	5.930	7.7095	19
2	1	0	.004459	.004459	.000000	7.658	7.658	5.9724	0
2	0	1	.005353	.005352	.000001	8.391	8.390	5.4512	1
2	1	1	.006239	.006243	-.000004	9.061	9.064	5.0490	19
3	0	1	.009811	.009811	.000000	11.369	11.369	4.0264	18
2	0	2	.010704	.010704	.000000	11.877	11.877	3.8548	14
3	2	0	.011593	.011594	-.000001	12.362	12.363	3.7041	3
3	2	1	.013376	.013378	-.000002	13.283	13.284	3.4483	2
4	0	0	.014269	.014270	-.000001	13.721	13.721	3.3387	2
3	0	2	.015164	.015163	.000001	14.147	14.147	3.2387	6
3	1	2	.016055	.016055	.000000	14.559	14.559	3.1475	14
4	1	1	.016947	.016946	.000001	14.960	14.959	3.0636	14
4	2	0	.017837	.017837	.000000	15.350	15.350	2.9862	7
3	2	2	.018727	.018730	-.000003	15.731	15.732	2.9143	0
2	0	3	.019625	.019624	.000001	16.106	16.106	2.8469	2
2	1	3	.020516	.020516	.000000	16.470	16.470	2.7844	2
4	0	2	.021411	.021406	.000005	16.828	16.826	2.7256	0
4	1	2	.022302	.022298	.000004	17.177	17.176	2.6706	0
3	0	3	.024085	.024084	.000001	17.856	17.856	2.5698	3

NUMBER OF OBS. LINES = 23

NUMBER OF CALC. LINES = 38

M(20)= 229

F 20 = 807

M(23)= 192

F 23 = 741

1 LINES ARE UNINDEXED

M-TEST= 229 UNINDEXED IN THE TEST= 1