

All indexations were done using the same procedure:

Peak hunting	- utility "peak search" from Winplotr (version June 2001).
Indexation	- Dicvol91, distributed with Winplotr (version June 2001).
Cell checking	- full-pattern fitting (Le Bail fit) with Fullprof2000
Cell reduction	- program LePage (version 30. October 1990)
Cell parameters refinement	- full-pattern fitting (Le Bail fit, sample 3) or Rietveld refinement (samples 1 and 2) with Fullprof2000
Systematic extinctions	- manual analysis
Space group determination	- based on systematic extinctions and Cryst. Tables, vol. A

Sample 1:

Crystal system : monoclinic

Cell parameters :

10.32131 0.00073
7.39292 0.00053
13.23675 0.00092
90.00000 0.00000
139.90027 0.00212
90.00000 0.00000

Possible space groups : $P2/c$ or Pc

The Bravais cell, which is given above, was obtained by the reduction of the cell with parameters $a=13.2237$ $b=14.7914$ $c= 8.5086$ $\beta=128.638$ found from the first 18 reflections with the figures of merit :

$$M(18) = 15.9$$

$$F(18) = 21.6$$

Indexed peaks for the cell $a=13.2237$ $b=14.7914$ $c= 8.5086$ $\beta=128.638$:

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
0	2	0	7.39436	7.39570	-0.00133	0.018290	0.01828	11.959	11.957	0.002
0	0	1	6.64976	6.64617	0.00359	0.022610	0.02264	13.304	13.311	-0.007
2	0	-1	6.49784	6.48904	0.00880	0.023680	0.02375	13.617	13.635	-0.019
2	0	0	5.16106	5.16456	-0.00350	0.037540	0.03749	17.167	17.155	0.012
0	2	1	4.94423	4.94337	0.00087	0.040910	0.04092	17.926	17.929	-0.003
2	2	-1	4.88095	4.87768	0.00327	0.041980	0.04203	18.160	18.173	-0.012
1	3	-1	4.26316	4.26568	-0.00252	0.055020	0.05496	20.820	20.807	0.012
1	2	1	3.82063	3.82121	-0.00058	0.068510	0.06849	23.263	23.259	0.004
3	2	-1	3.76016	3.76076	-0.00060	0.070730	0.07070	23.642	23.639	0.004
0	4	0	3.69738	3.69785	-0.00047	0.073150	0.07313	24.050	24.047	0.003
0	0	2	3.32452	3.32308	0.00144	0.090480	0.09056	26.795	26.806	-0.012
0	4	1	3.23016	3.23136	-0.00120	0.095840	0.09577	27.593	27.582	0.010
2	4	-1	3.21486	3.21280	0.00206	0.096760	0.09688	27.727	27.745	-0.018
4	0	-1	3.16308	3.16479	-0.00171	0.099950	0.09984	28.190	28.174	0.016
4	2	-1	2.91067	2.90958	0.00108	0.118040	0.11812	30.692	30.704	-0.012
3	0	-3	2.83430	2.83537	-0.00107	0.124480	0.12439	31.540	31.528	0.012
4	0	0	2.58239	2.58228	0.00011	0.149950	0.14997	34.710	34.711	-0.001
4	2	-3	2.55061	2.55065	-0.00004	0.153710	0.15371	35.156	35.156	0.001

Sample 2:

Crystal system : monoclinic

Cell parameters :

11.24284 0.00002
8.19537 0.00002
19.94842 0.00004
90.00000 0.00000
106.72856 0.00017
90.00000 0.00000

Possible space groups : $P2_1/c$

The Bravais cell, which is given above, was found from the first 20 reflections with the figures of merit :

$$M(20) = 155.5$$

$$F(20) = 777.1$$

Indexed peaks for the cell in the setting $a=19.8806$ $b=8.1947$ $c=11.2419$ $\beta=106.072$:

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
1	0	-1	10.76690	10.76665	0.00026	0.008630	0.00863	4.246	4.246	0.000
2	0	0	9.55167	9.55182	-0.00014	0.010960	0.01096	4.786	4.786	0.000
1	0	1	8.45464	8.45379	0.00084	0.013990	0.01399	5.407	5.408	-0.001
1	1	0	7.53199	7.53105	0.00094	0.017630	0.01763	6.070	6.071	-0.001
0	1	1	6.52417	6.52873	-0.00456	0.023490	0.02346	7.009	7.004	0.005
1	1	-1		6.52079	0.00338		0.02352		7.013	-0.004
2	1	0	6.21952	6.21949	0.00003	0.025850	0.02585	7.353	7.353	0.000
1	1	1	5.88208	5.88399	-0.00192	0.028900	0.02888	7.776	7.773	0.003
0	0	2	5.40040	5.40124	-0.00084	0.034290	0.03428	8.470	8.469	0.001
2	0	-2	5.38385	5.38332	0.00052	0.034500	0.03451	8.496	8.497	-0.001
3	1	0	5.02815	5.02821	-0.00007	0.039550	0.03955	9.099	9.099	0.000
3	0	1	4.92207	4.92191	0.00017	0.041280	0.04128	9.295	9.295	0.000
4	0	0	4.77570	4.77591	-0.00021	0.043850	0.04384	9.581	9.580	0.000
1	1	-2	4.63524	4.63523	0.00001	0.046540	0.04654	9.872	9.872	0.000
2	0	2	4.22714	4.22690	0.00024	0.055960	0.05597	10.828	10.828	-0.001
4	1	-1	4.20134	4.20440	-0.00306	0.056650	0.05657	10.894	10.886	0.008
4	0	-2		4.20124	0.00010		0.05666		10.894	0.000
1	1	2	4.17875	4.17846	0.00029	0.057270	0.05728	10.953	10.954	-0.001
3	1	-2	4.16177	4.16189	-0.00012	0.057740	0.05773	10.998	10.998	0.000
4	1	0	4.12632	4.12628	0.00005	0.058730	0.05873	11.093	11.093	0.000
0	2	0	4.09747	4.09735	0.00012	0.059560	0.05957	11.171	11.172	0.000
1	2	0	4.00627	4.00624	0.00004	0.062300	0.06231	11.426	11.426	0.000

Sample 3:

Crystal system : cubic

Cell parameters :

18.87892 0.00004
 18.87892 0.00004
 18.87892 0.00004
 90.00000 0.00000
 90.00000 0.00000
 90.00000 0.00000

Possible space groups : $I23$, $I2_13$, $Im-3$, $I432$, $I-43m$, $Im-3m$

The Bravais cell was found from the first 25 reflections with the figures of merit :

$$M(25) = 75.3$$

$$F(25) = 222.5$$

Indexed peaks :

H	K	L	DOBS	DCAL	DOBS-DCAL	QOBS	QCAL	2TH.OBS	2TH.CAL	DIF.2TH.
1	1	0	13.38535	13.35431	0.03105	0.005580.00561		3.415	3.423	-0.008
2	0	0	9.45163	9.44292	0.00871	0.011190.01121		4.837	4.841	-0.004
2	1	1	7.71473	7.71011	0.00461	0.016800.01682		5.927	5.930	-0.004
3	1	0	5.97491	5.97223	0.00268	0.028010.02804		7.655	7.658	-0.003
2	2	2	5.45266	5.45187	0.00079	0.033630.03364		8.389	8.390	-0.001
3	2	1	5.04837	5.04745	0.00092	0.039240.03925		9.062	9.064	-0.002
4	0	0	4.72246	4.72146	0.00100	0.044840.04486		9.689	9.691	-0.002
3	3	0	4.45203	4.45144	0.00060	0.050450.05047		10.279	10.280	-0.001
4	1	1		4.45144	0.00060	0.05047			10.280	-0.001
3	3	2	4.02681	4.02647	0.00034	0.061670.06168		11.368	11.369	-0.001
4	2	2	3.85524	3.85506	0.00018	0.067280.06729		11.876	11.876	-0.001
4	3	1	3.70395	3.70382	0.00013	0.072890.07290		12.363	12.363	0.000
5	1	0		3.70382	0.00013	0.07290			12.363	0.000
5	2	1	3.44813	3.44807	0.00007	0.084110.08411		13.284	13.284	0.000
4	4	0	3.33837	3.33858	-0.00020	0.089730.08972		13.722	13.722	0.001
4	3	3	3.23887	3.23890	-0.00003	0.095330.09532		14.146	14.146	0.000
5	3	0		3.23890	-0.00003	0.09532			14.146	0.000
4	4	2	3.14756	3.14764	-0.00008	0.100940.10093		14.559	14.558	0.000
6	0	0		3.14764	-0.00008	0.10093			14.558	0.000
5	3	2	3.06363	3.06369	-0.00006	0.106540.10654		14.960	14.960	0.000
6	1	1		3.06369	-0.00006	0.10654			14.960	0.000
6	2	0	2.98600	2.98611	-0.00011	0.112160.11215		15.351	15.351	0.001
5	4	1	2.91404	2.91415	-0.00011	0.117760.11775		15.733	15.732	0.001
6	2	2	2.84702	2.84715	-0.00013	0.123370.12336		16.105	16.105	0.001
6	3	1	2.78440	2.78457	-0.00017	0.128980.12897		16.470	16.469	0.001
4	4	4	2.72580	2.72594	-0.00013	0.134590.13458		16.827	16.826	0.001
5	4	3	2.67069	2.67086	-0.00017	0.140200.14018		17.176	17.175	0.001
5	5	0		2.67086	-0.00017	0.14018			17.175	0.001
7	1	0		2.67086	-0.00017	0.14018			17.175	0.001
6	4	0	2.61887	2.61900	-0.00013	0.145810.14579		17.519	17.518	0.001
5	5	2	2.56984	2.57004	-0.00020	0.151420.15140		17.856	17.855	0.001
6	3	3		2.57004	-0.00020	0.15140			17.855	0.001
7	2	1		2.57004	-0.00020	0.15140			17.855	0.001
6	4	2	2.52317	2.52373	-0.00056	0.157080.15701		18.189	18.185	0.004