

## Unit-cell indexing

### ORTHORHOMBIC SYSTEM

DIRECT PARAMETERS : A= 12.90347 B= 8.97075 C= 4.79267 VOLUME= 554.77  
STANDARD DEVIATIONS : 0.00088 0.00050 0.00024

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

2	0	1	3.84657	3.84730	-0.00074	23.095	23.090	0.004
2	2	0	3.68206	3.68281	-0.00075	24.142	24.137	0.005
2	1	1	3.53571	3.53584	-0.00014	25.157	25.156	0.001
4	0	0	3.22545	3.22587	-0.00042	27.623	27.619	0.004
3	0	1	3.20086	3.20109	-0.00023	27.839	27.837	0.002
1	2	1	3.17373	3.17425	-0.00052	28.082	28.077	0.005
4	1	0	3.03532	3.03557	-0.00025	29.391	29.388	0.002
3	1	1	3.01460	3.01489	-0.00029	29.597	29.594	0.003
2	3	0	2.71297	2.71302	-0.00005	32.977	32.976	0.001
4	2	0	2.61887	2.61890	-0.00003	34.198	34.197	0.000
3	2	1	2.60591	2.60559	0.00032	34.373	34.377	-0.004
4	1	1	2.56441	2.56445	-0.00004	34.947	34.946	0.001
0	3	1	2.53674	2.53696	-0.00022	35.341	35.337	0.003
1	3	1	2.48907	2.48930	-0.00023	36.040	36.037	0.003
0	0	2	2.39607	2.39634	-0.00027	37.490	37.486	0.004
2	3	1	2.36080	2.36098	-0.00018	38.072	38.069	0.003
1	0	2	2.35600	2.35605	-0.00005	38.152	38.151	0.001
4	2	1	2.29839	2.29817	0.00022	39.147	39.151	-0.004
1	1	2	2.27911	2.27877	0.00034	39.492	39.498	-0.006
2	0	2	2.24658	2.24639	0.00019	40.088	40.092	-0.004
0	4	0	2.24270	2.24269	0.00002	40.160	40.161	0.000
4	3	0	2.19338	2.19300	0.00038	41.104	41.111	-0.007
3	3	1	2.18549	2.18516	0.00033	41.259	41.265	-0.006

#### \* NUMBER OF LINES

.- INPUT DATA = 23  
.- CALCULATED = 50

#### \* MEAN ABSOLUTE DISCREPANCIES

<Q> =0.2694E-04  
<DELTA(2-THETA)> =0.3262E-02  
MAX. ERROR ACCEPTED (DEG. 2-THETA) =0.3500E-01

#### \* FIGURES OF MERIT

1.- M( 23) = 77.7 (REF. 4)  
2.- F( 23) = 141.0(0.0033, 50) (REF. 5)

=====> CELL VOLUME = 554.8 A\*\*3 M(23)= 77.7 F(23)= 141.0(0.0033, 50)

#### DICVOL : Useful References

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- 1 D. Louër & M. Louër (1972). J. Appl. Cryst. 5, 271-275.
- 2 A. Boultif & D. Louër (1991). J. Appl. Cryst. 24, 987-993.
- 3 D. Louër & R. Vargas (1982). J. Appl. Cryst. 15, 542-545.
- 4 P.M. de Wolff (1968). J. Appl. Cryst. 5, 108-113.
- 5 G.S. Smith & R.L. Snyder (1979). J. Appl. Cryst. 12, 60-65.