

Tableau IV.1 : Fichier.out pour le composé Ca(C₂O₄).H₂O

```

1 -----
| caox |
-----
                                INPUT DATA
                                *****

EXPERIMENTAL                    EXPERIMENTAL
 2-THETA                          ERROR

14.902                          0.040
15.223                          0.040
19.526                          0.040
23.451                          0.040
23.523                          0.040
23.660                          0.040
24.360                          0.040
29.645                          0.040
30.077                          0.040
30.726                          0.040
35.471                          0.040
35.850                          0.040
36.484                          0.040
36.732                          0.040
37.273                          0.040
37.436                          0.040
38.144                          0.040
39.739                          0.040

*****

----- PARAMETER LIMITS -----
| A MAXIMUM      = 30.00 A |
| B MAXIMUM      = 30.00 A |
| C MAXIMUM      = 30.00 A |
| BETA MINIMUM   = 90.00 Deg. |
| BETA MAXIMUM   = 125.00 Deg. |
-----

----- VOLUME LIMITS -----
| VOLUME MINIMUM = 0.00 A**3 |
| VOLUME MAXIMUM = 4000.00 A**3 |
-----

                                WAVELENGTH = 1.540598 A
LOWER FIGURE OF MERIT REQUIRED FOR PRINTED SOLUTION(S) : M( 18) = 10.0
MAXIMUM NUMBER OF ACCEPTED UNINDEXED LINES AMONG THE FIRST 18 INPUT LINES: 0
*****
**
** ATTENTION : VOS DONNEES SONT-ELLES IRREPROCHABLES ? **
** WARNING : ARE YOUR DATA IRREPROACHABLE ? **
**
*****

SEARCH OF MONOCLINIC SOLUTION(S)
*****

SEARCH OF MONOCLINIC SOLUTION(S) WITHIN THE LIMITS ON LINEAR PARAMETERS
*****
(SLIGHT TOLERANCE ACCEPTED): AMAX= 12.412 BMAX= 12.412 CMAX= 12.412

VOLUME DOMAIN BEING SCANNED :
=====
LOWER BOUND = 0.00 A**3 HIGHER BOUND = 400.00 A**3
ANGLE RANGE SCANNED : BETA MIN= 90.000 Deg. BETA MAX= 95.000 Deg.
ANGLE RANGE SCANNED : BETA MIN= 95.000 Deg. BETA MAX=100.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=100.000 Deg. BETA MAX=105.000 Deg.

```

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

DIRECT PARAMETERS : A=12.0565 B= 4.9229 C= 6.0741 BETA=102.062 VOLUME= 352.56
 STANDARD DEVIATIONS : 0.0028 0.0008 0.0013 0.024
 REDUCED CELL : A= 6.0741 B= 4.9229 C=12.0565 BETA=102.062 VOLUME= 352.56

H	K	L	DOBS	DCAL	DOBS-DCAL	2TH.OBS	2TH.CAL	DIF.2TH.
0	0	1	5.94008	5.93996	0.00011	14.902	14.902	0.000
1	0	-1	5.81554	5.81552	0.00001	15.223	15.223	0.000
1	1	0	4.54258	4.54284	-0.00027	19.526	19.525	0.001
0	1	1	3.79041	3.79038	0.00003	23.451	23.451	0.000
2	1	0	3.77897	3.77866	0.00031	23.523	23.525	-0.002
1	1	-1	3.75740	3.75743	-0.00003	23.660	23.660	0.000
3	0	-1	3.65099	3.64707	0.00392	24.360	24.387	-0.027
2	1	1	3.01103	3.01082	0.00022	29.645	29.647	-0.002
0	0	2	2.96876	2.96998	-0.00122	30.077	30.064	0.013
2	0	-2	2.90752	2.90776	-0.00024	30.726	30.723	0.003
4	1	0	2.52869	2.52893	-0.00024	35.471	35.468	0.003
2	1	-2	2.50283	2.50365	-0.00082	35.850	35.838	0.012
0	2	0	2.46077	2.46147	-0.00070	36.484	36.473	0.011
4	0	1	2.44473	2.44477	-0.00004	36.732	36.731	0.001
1	2	0	2.41048	2.40952	0.00096	37.273	37.288	-0.015
1	1	2	2.40035	2.39897	0.00138	37.436	37.458	-0.022
5	0	0	2.35741	2.35807	-0.00066	38.144	38.133	0.011
1	2	-1	2.26639	2.26679	-0.00039	39.739	39.732	0.007

* NUMBER OF LINES

.- LINES INPUT = 18
 .- LINES INDEXED = 18
 .- LINES CALCULATED = 45

* MEAN ABSOLUTE DISCREPANCIES

<Q> =0.5825E-04
 <DELTA(2-THETA)> =0.7263E-02
 MAX. ERROR ACCEPTED (DEG. 2-THETA) =0.5500E-01

* FIGURES OF MERIT

1.- M(18) = 37.1
 2.- F(18) = 55.1(0.0073, 45)

ANGLE RANGE SCANNED : BETA MIN=105.000 Deg. BETA MAX=110.000 Deg.
 ANGLE RANGE SCANNED : BETA MIN=110.000 Deg. BETA MAX=115.000 Deg.
 ANGLE RANGE SCANNED : BETA MIN=115.000 Deg. BETA MAX=120.000 Deg.
 ANGLE RANGE SCANNED : BETA MIN=120.000 Deg. BETA MAX=125.000 Deg.

ITERATION NUMBER AT EACH DICHOTOMY LEVEL :

1139 939 272 46 36 49 120

END OF SEARCH FOR MONOCLINIC SOLUTIONS

 --- T O T A L CALCULATION TIME : 0.500 SEC
 DICVOL91 : USEFUL REFERENCES

- * LOUER, D. & LOUER, M. (1972). J. APPL. CRYST. 5, 271-275.
 * BOULTIF, A. & LOUER, D. (1991). J. APPL. CRYST. 24, 987-993.

Tableau IV.2 : Fichier de sortie PDFEAPC .out graphique du programme NBS*AIDS83

```

JCFDS - ICDD  ** Edit Aids PC-90 **      Revision pc      90/02/28
Numerical Analysis Run
PARAMETERS as INPUT:
      IJOB = 0          INCODN = 0          IBK = 0
      IWHO = 0          IOUT = 2           IINPUT = 0
      IFRMT = 0         ITHMX = 0          ICOL = 0
      IXCD = 0          IXPD = 0           IPHKL = 0
                        IDOLSQ = 2

.....
      *** MONOCLINIC ***      ***      :6/ 8/29      9:31:50
0.....1.....2.....3.....4.....5.....6.....7.
12.0565  4.9229  6.0741          102.062          CELL 1
                        7E B          ESDS 2
P 2/m      0          352.56      SG-I 3
P 2/m      0          352.56      SG-F 4
I          FLGS 5
T-2      .00 1.00 .00 / .00 .00 1.00 / 1.00 .00 .00      MATX
1.00: 1.00 .00 .00 / .00 1.00 .00 / .00 .00 1.00      MATX C
      12.057  4.923  6.074  90.00 102.06  90.00  352.56      C-IN
      4.923  6.074  12.057 102.06  90.00  90.00  352.56      35      C-RD D
      12.057  4.923  6.074  90.00 102.06  90.00  2.4491 1.2338      C-CD E
      24.235 36.895 145.359 -15.303 .000 .000      DOTM
      1.5406          2          PDF1 F
      :6/ 8/29 0 0 pc 90/02/28          HIST K
      A          B          C          Alpha          Beta          Gamma          VOLUME
      RECIPROCAL CELL
      .84815E-01 .20313E+00 .16835E+00  89.99999  77.93800  89.99999 .283643E-02
      DIRECT CELL
      12.056500  4.922900  6.074100  90.00000 102.06200  90.00000 .352556E+03
1-THETA ANGLES      THMX = 20.0  NCYC = 2  TOLMN = .0250  TOLMX = .1000
      THEMX = 20.4  DMIN = 2.213049  LAMBDA =1.5406000
      0 CONDITIONS for NON-EXTINCTION requested
      Cycle 1
      2-Theta TOLERANCE = .20000
      N  H  K  L  D calc  D obs  Lambda  2-é calc  2-é obs  2-é DIFF  WT
      1  -1  0  1  5.81554  5.81555  1.540600  15.22301  15.22300  .00001  1.00
      2  -1  1  0  4.54281  4.54258  1.540600  19.52501  19.52600  -.00098  1.00
      3  -3  0  1  3.64707  3.65099  1.540600  24.38663  24.36000  .02663  1.00
      4  0  0  2  2.97000  2.96877  1.540600  30.06423  30.07700  -.01277  1.00
      5  -4  1  0  2.52892  2.52870  1.540600  35.46772  35.47100  -.00328  1.00
      LARGEST RESIDUAL reduced to UNIT WEIGHT .02663 for OBS 3
      STANDARD ERROR UNIT WT for OBS .00876 with DEGREES of FREEDOM 1
      A          B          C          Alpha          Beta          Gamma          VOLUME
      RECIPROCAL CELL
      .84815E-01 .20316E+00 .16843E+00  90.0000  77.8303  90.0000 .283703E-02
      R C CORRECTIONS
      -.32047E-06 .26762E-04 .82319E-04 .0000  -.1077  .0000 .605360E-06
      DIRECT CELL
      12.061410  4.922252  6.073581  90.0000 102.1697  90.0000 352.481000
      D C CORRECTIONS
      .004910  -.000648  -.000519 .0000  .1077  .0000  -.075226
      Cycle 2
      2-Theta TOLERANCE = .05000
      N  H  K  L  D calc  D obs  Lambda  2-é calc  2-é obs  2-é DIFF  WT
      1  0  0  1  5.93709  5.94009  1.540600  14.90955  14.90200  .00755  1.00
      2  -1  0  1  5.81827  5.81555  1.540600  15.21582  15.22300  -.00718  1.00
      3  -1  1  0  4.54230  4.54258  1.540600  19.52722  19.52600  .00122  1.00
      4  0  1  1  3.78932  3.79042  1.540600  23.45790  23.45100  -.00690  1.00
      5  2  1  0  3.77835  3.77898  1.540600  23.52695  23.52300  .00395  1.00
      6  -1  1  1  3.75787  3.75740  1.540600  23.65705  23.66000  -.00295  1.00
      7  -3  0  1  3.65044  3.65099  1.540600  24.36374  24.36000  .00373  1.00
      8  2  1  1  3.00878  3.01104  1.540600  29.66776  29.64500  .02275  1.00
      9  0  0  2  2.96855  2.96877  1.540600  30.07928  30.07700  .00228  1.00
      10 -2  0  2  2.90914  2.90752  1.540600  30.70854  30.72600  -.01746  1.00
      11 -4  1  0  2.52884  2.52870  1.540600  35.46889  35.47100  -.00211  1.00
      12 -2  1  2  2.50443  2.50283  1.540600  35.82624  35.85000  -.02376  1.00
      13  0  2  0  2.46113  2.46078  1.540600  36.47865  36.48400  -.00536  1.00
      14  4  0  1  2.44296  2.44473  1.540600  36.75960  36.73200  .02760  1.00
      15  1  2  0  2.40920  2.41048  1.540600  37.29355  37.27300  .02055  1.00
      16  1  1  2  2.39738  2.40036  1.540600  37.48429  37.43600  .04829  1.00
      17 -1  2  1  2.26668  2.26640  1.540600  39.73381  39.73900  -.00519  1.00
      LARGEST RESIDUAL reduced to UNIT WEIGHT .04829 for OBS 16
      STANDARD ERROR UNIT WT for OBS .01190 with DEGREES of FREEDOM 13
      A          B          C          Alpha          Beta          Gamma          VOLUME
      RECIPROCAL CELL
  
```

```

.84795E-01 .20314E+00 .16836E+00 90.0000 77.9348 90.0000.283592E-02
R C CORRECTIONS
-.19692E-04-.23931E-04-.72818E-04 .0000 .1045 .0000*****
DIRECT CELL
12.059490 4.922832 6.073831 90.0000 102.0652 90.0000 352.618900
D C CORRECTIONS
-.001921 .000580 .000249 .0000 -.1045 .0000 .137878
Cycle 3
2-Theta TOLERANCE = .05000
N H K L D calc D obs Lambda 2-é calc 2-é obs 2-é DIFF WT
1 0 0 1 5.93966 5.94009 1.540600 14.90307 14.90200 .00107 1.00
2 -1 0 1 5.81561 5.81555 1.540600 15.22282 15.22300 -.00018 1.00
3 -1 1 0 4.54292 4.54258 1.540600 19.52456 19.52600 -.00144 1.00
4 0 1 1 3.79025 3.79042 1.540600 23.45205 23.45100 .00105 1.00
5 2 1 0 3.77897 3.77898 1.540600 23.52302 23.52300 .00002 1.00
6 -1 1 1 3.75741 3.75740 1.540600 23.65998 23.66000 -.00002 1.00
7 -3 0 1 3.64777 3.65099 1.540600 24.38188 24.36000 .02188 1.00
8 2 1 1 3.01093 3.01104 1.540600 29.64612 29.64500 .00112 1.00
9 0 0 2 2.96983 2.96877 1.540600 30.06597 30.07700 -.01103 1.00
10 -2 0 2 2.90781 2.90752 1.540600 30.72293 30.72600 -.00307 1.00
11 -4 1 0 2.52935 2.52870 1.540600 35.46149 35.47100 -.00951 1.00
12 -2 1 2 2.50366 2.50283 1.540600 35.83767 35.85000 -.01233 1.00
13 0 2 0 2.46142 2.46078 1.540600 36.47419 36.48400 -.00981 1.00
14 4 0 1 2.44513 2.44473 1.540600 36.72578 36.73200 -.00622 1.00
15 1 2 0 2.40949 2.41048 1.540600 37.28881 37.27300 .01581 1.00
16 1 1 2 2.39890 2.40036 1.540600 37.45960 37.43600 .02360 1.00
17 5 0 0 2.35862 2.35742 1.540600 38.12378 38.14400 -.02023 1.00
18 -1 2 1 2.26675 2.26640 1.540600 39.73254 39.73900 -.00645 1.00
LARGEST RESIDUAL reduced to UNIT WEIGHT .02360 for OBS 16
STANDARD ERROR UNIT WT for OBS .01214 with DEGREES of FREEDOM 14
A B C Alpha Beta Gamma VOLUME
RECIPROCAL CELL
.84815E-01 .20313E+00 .16835E+00 90.0000 77.9379 90.0000.283640E-02
R C CORRECTIONS
.19724E-04-.47778E-05-.87651E-05 .0000 .0031 .0000.478234E-06
DIRECT CELL
12.056550 4.922947 6.074076 90.0000 102.0621 90.0000 352.559500
D C CORRECTIONS
-.002944 .000115 .000245 .0000 -.0031 .0000 -.059448
Cycle 4
2-Theta TOLERANCE = .05000
N H K L D calc D obs Lambda 2-é calc 2-é obs 2-é DIFF WT
1 0 0 1 5.93997 5.94009 1.540600 14.90229 14.90200 .00029 1.00
2 -1 0 1 5.81553 5.81555 1.540600 15.22304 15.22300 .00004 1.00
3 -1 1 0 4.54285 4.54258 1.540600 19.52484 19.52600 -.00116 1.00
4 0 1 1 3.79038 3.79042 1.540600 23.45122 23.45100 .00022 1.00
5 2 1 0 3.77866 3.77898 1.540600 23.52497 23.52300 .00197 1.00
6 -1 1 1 3.75744 3.75740 1.540600 23.65979 23.66000 -.00021 1.00
7 -3 0 1 3.64708 3.65099 1.540600 24.38657 24.36000 .02657 1.00
8 2 1 1 3.01082 3.01104 1.540600 29.64717 29.64500 .00217 1.00
9 0 0 2 2.96999 2.96877 1.540600 30.06436 30.07700 -.01264 1.00
10 -2 0 2 2.90776 2.90752 1.540600 30.72337 30.72600 -.00263 1.00
11 -4 1 0 2.52894 2.52870 1.540600 35.46753 35.47100 -.00347 1.00
12 -2 1 2 2.50365 2.50283 1.540600 35.83783 35.85000 -.01217 1.00
13 0 2 0 2.46147 2.46078 1.540600 36.47331 36.48400 -.01069 1.00
14 4 0 1 2.44477 2.44473 1.540600 36.73133 36.73200 -.00067 1.00
15 1 2 0 2.40952 2.41048 1.540600 37.28831 37.27300 .01531 1.00
16 1 1 2 2.39898 2.40036 1.540600 37.45834 37.43600 .02234 1.00
17 5 0 0 2.35807 2.35742 1.540600 38.13299 38.14400 -.01101 1.00
18 -1 2 1 2.26679 2.26640 1.540600 39.73181 39.73900 -.00719 1.00
LARGEST RESIDUAL reduced to UNIT WEIGHT .02657 for OBS 7
STANDARD ERROR UNIT WT for OBS .01214 with DEGREES of FREEDOM 14
A B C Alpha Beta Gamma VOLUME
RECIPROCAL CELL
.84815E-01 .20313E+00 .16835E+00 90.0000 77.9379 90.0000.283640E-02
R C STNRD ERRS
.17534E-04 .35053E-04 .36921E-04 .0000 .0243 .0000
R C CORRECTIONS
-.37514E-08-.31450E-09 .48812E-08 .0000 .0000 .0000*****
DIRECT CELL
12.056550 4.922947 6.074076 90.0000 102.0621 90.0000 352.559500
D C STNRD ERRS
.002831 .000850 .001265 .0000 .0243 .0000 .098310
D C CORRECTIONS
.000001 .000000 .000000 .0000 .0000 .0000 .000031
DIRECT CELL VARIANCE-COVARIANCE MATRIX ROW
.801262E-05-.263895E-06-.421732E-06 .000000E+00 .581172E-06 .000000E+00 1
-.263895E-06 .721685E-06-.216446E-06 .000000E+00-.283611E-08 .000000E+00 2

```

-.421732E-06-.216446E-06 .159951E-05 .000000E+00 .494035E-07 .000000E+00 3
 .000000E+00 .000000E+00 .000000E+00 .000000E+00 .000000E+00 .000000E+00 4
 .581172E-06-.283611E-08 .494035E-07 .000000E+00 .179999E-06 .000000E+00 5
 .000000E+00 .000000E+00 .000000E+00 .000000E+00 .000000E+00 .000000E+00 6

DIRECT CELL CORRELATION MATRIX ROW
 1.000000 -.109741 -.117803 .000000 .483929 .000000 1
 -.109741 1.000000 -.201457 .000000 -.007869 .000000 2
 -.117803 -.201457 1.000000 .000000 .092072 .000000 3
 .000000 .000000 .000000 .000000 .000000 .000000 4
 .483929 -.007869 .092072 .000000 1.000000 .000000 5
 .000000 .000000 .000000 .000000 .000000 .000000 6

N		D calc		D obs		INT	H K L			OBS			CALC		DIFF		FINL		WT
													2Theta		2Theta				
1	11.7904									1	0	0	14.902	14.902	.000	7.492			
2	5.9400	5.9401	0	0	0	1C	0	0	1	2	0	0	14.902	14.902	.000	15.016			1.0
4	5.8155	5.8155	0	-1	0	1C	-1	0	1	0	1	0	15.223	15.223	.000	18.004			1.0
	5	4.9229								1	0	1	18.057			18.847			
	6	4.9086								1	0	1	18.057			18.847			
	7	4.7046								-2	0	1	19.526	19.525	-.001	22.606			1.0
8	4.5428	4.5426	0	-1	1	0C	-1	1	0	3	0	0	19.526	19.525	-.001	23.357			1.0
	9	3.9301								2	0	1	23.451	23.451	.000	23.523			1.0
	10	3.8055								2	0	1	23.451	23.451	.000	23.525			1.0
11	3.7904	3.7904	0	0	1	1C	0	1	1	0	1	0	23.523	23.525	.002	23.660			1.0
12	3.7787	3.7790	0	2	1	0C	2	1	0	1	1	1	23.660	23.660	.000	24.360			1.0
13	3.7574	3.7574	0	-1	1	1C	-1	1	1	1	1	1	24.360	24.387	.027	25.607			1.0
14	3.6471	3.6510	0	-3	0	1C	-3	0	1	1	1	1	24.360	24.387	.027	26.180			1.0
	15	3.4760								-2	1	1	25.607			26.180			
	16	3.4012								3	1	0	26.180			29.049			
	17	3.0714								-1	0	2	29.049			29.414			
	18	3.0341								3	0	1	29.414			29.647			1.0
19	3.0108	3.0110	0	2	1	1C	2	1	1	3	0	1	29.645	29.647	.002	29.740			1.0
	20	3.0017								3	0	1	29.740			30.077			1.0
21	2.9700	2.9688	0	0	0	2C	0	0	2	4	0	0	30.077	30.064	-.013	30.298			1.0
	22	2.9476								-3	1	1	30.298			30.479			
	23	2.9305								-3	1	1	30.479			30.726			1.0
24	2.9078	2.9075	0	-2	0	2C	-2	0	2	-4	0	1	30.726	30.723	-.003	30.896			1.0
	25	2.8920								1	0	2	30.896			32.567			
	26	2.7472								-3	0	2	32.567			33.786			
	27	2.6509								-1	1	2	33.786			34.702			
	28	2.5829								3	1	1	34.702			34.983			
	29	2.5628								0	1	2	34.983			35.264			
	30	2.5430								0	1	2	35.264			35.468			1.0
31	2.5289	2.5287	0	-4	1	0C	-4	1	0	35.471	35.468	-.003	35.471	35.468	-.003	35.838			1.0
32	2.5037	2.5028	0	-2	1	2C	-2	1	2	-4	1	1	35.838	35.838	-.012	35.988			1.0
	33	2.4935								2	0	2	35.988			36.473			1.0
34	2.4615	2.4608	0	0	2	0C	0	2	0	2	0	2	36.473	36.473	-.011	36.584			1.0
	35	2.4543								2	0	2	36.584			36.732			1.0
36	2.4448	2.4447	0	4	0	1C	4	0	1	36.732	36.731	-.001	36.732	36.731	-.001	37.273			1.0
37	2.4095	2.4105	0	1	2	0C	1	2	0	37.273	37.288	.015	37.273	37.288	.015	37.436			1.0
38	2.3990	2.4004	0	1	1	2C	1	1	2	37.436	37.458	.022	37.436	37.458	.022	37.968			1.0
	39	2.3679								-5	0	1	37.968			38.133			1.0
40	2.3581	2.3574	0	5	0	0C	5	0	0	-4	0	2	38.133	38.133	-.011	38.230			1.0
	41	2.3523								-3	1	2	38.230			38.541			
	42	2.3340								0	2	1	38.541			39.601			
	43	2.2740								-2	2	0	39.601			39.647			
	44	2.2714								39.739	39.732	-.007	39.739	39.732	-.007				1.0
45	2.2668	2.2664	0	-1	2	1C	-1	2	1										

REFLECTION SUMMARY for ENTIRE PATTERN:
 ESTIMATED RESOLUTION = .075 deg 2-Theta
 THEORETICAL # of LINES = 45
 THEORETICAL RESOLVABLE = 42
 UNIQUE OBSERVED LINES = 18
 TOTAL LINES INPUT= 18
 NUMBER INDEXED= 18
 NUMBER UNINDEXED= 0
 NUMBER FLAGGED = 0

***** FOR INDEXED LINES *****

AVERAGE 2-Theta DIFFERENCE = .000

with DIFF > +0.05(2-Theta) = 0

with DIFF < -0.05(2-Theta) = 0

C/SIGMA (NON-RANDOM ERROR TEST) = .81

M(18) = 37.3 (DLIMIT = 2.2609, # POSSIBLE = 45)

X(18) = 0

F(18) = 55.1 (DELTA 2-Theta = .0073, # POSSIBLE = 45)

Tableau V.1 : Fichier.out pour le composé CaZr(C₂O₄)₃.9H₂O

1

ZrCaOx

INPUT DATA

EXPERIMENTAL 2-THETA	EXPERIMENTAL ERROR
12.519	0.020
13.100	0.020
15.714	0.020
20.511	0.020
23.853	0.020
25.945	0.020
31.731	0.020
32.868	0.020
37.900	0.020
40.023	0.020
41.544	0.020
42.971	0.020
43.250	0.020
45.918	0.020
46.345	0.020
48.829	0.020
55.004	0.020
57.073	0.020
57.580	0.020
57.740	0.020

PARAMETER LIMITS	VOLUME LIMITS
A MAXIMUM = 30.00 A	VOLUME MINIMUM = 0.00 A**3
B MAXIMUM = 30.00 A	VOLUME MAXIMUM = 2000.00 A**3
C MAXIMUM = 30.00 A	
BETA MINIMUM = 90.00 Deg.	
BETA MAXIMUM = 125.00 Deg.	

 WAVELENGTH = 1.540598 A

LOWER FIGURE OF MERIT REQUIRED FOR PRINTED SOLUTION(S) : M(20) = 10.0
 MAXIMUM NUMBER OF ACCEPTED UNINDEXED LINES AMONG THE FIRST 20 INPUT LINES: 0

 **
 ** ATTENTION : VOS DONNEES SONT-ELLES IRREPROCHABLES ? **
 ** WARNING : ARE YOUR DATA IRREPROACHABLE ? **
 **

SEARCH OF MONOCLINIC SOLUTION(S)

SEARCH OF MONOCLINIC SOLUTION(S) WITHIN THE LIMITS ON LINEAR PARAMETERS

 (SLIGHT TOLERANCE ACCEPTED): AMAX= 14.652 BMAX= 14.652 CMAX= 14.652

VOLUME DOMAIN BEING SCANNED :

=====

LOWER BOUND =	0.00 A**3	HIGHER BOUND =	400.00 A**3
ANGLE RANGE SCANNED :	BETA MIN= 90.000 Deg.	BETA MAX=	95.000 Deg.
ANGLE RANGE SCANNED :	BETA MIN= 95.000 Deg.	BETA MAX=	100.000 Deg.
ANGLE RANGE SCANNED :	BETA MIN=100.000 Deg.	BETA MAX=	105.000 Deg.
ANGLE RANGE SCANNED :	BETA MIN=105.000 Deg.	BETA MAX=	110.000 Deg.
ANGLE RANGE SCANNED :	BETA MIN=110.000 Deg.	BETA MAX=	115.000 Deg.
ANGLE RANGE SCANNED :	BETA MIN=115.000 Deg.	BETA MAX=	120.000 Deg.
ANGLE RANGE SCANNED :	BETA MIN=120.000 Deg.	BETA MAX=	125.000 Deg.

ITERATION NUMBER AT EACH DICHOTOMY LEVEL :

439 510 220 12 0 0 0

NO SOLUTION
VOLUME DOMAIN BEING SCANNED :

=====

LOWER BOUND = 400.00 A**3 HIGHER BOUND = 800.00 A**3
ANGLE RANGE SCANNED : BETA MIN= 90.000 Deg. BETA MAX= 95.000 Deg.
ANGLE RANGE SCANNED : BETA MIN= 95.000 Deg. BETA MAX=100.000 Deg.
M O N O C L I N I C S Y S T E M
DIRECT PARAMETERS : A= 9.1124 B=11.2708 C= 6.7860 BETA= 95.692 VOLUME= 693.51
STANDARD DEVIATIONS : 0.0003 0.0005 0.0003 0.004

REDUCED CELL : A= 6.7860 B=11.2708 C= 9.1124 BETA= 95.692 VOLUME= 693.51

H	K	L	DOBS	DCAL	DOBS-DCAL	2TH.OBS	2TH.CAL	DIF.2TH.
1	1	0	7.06491	7.06491	-0.00001	12.519	12.519	0.000
0	0	1	6.75285	6.75257	0.00028	13.100	13.101	-0.001
0	2	0	5.63491	5.63539	-0.00048	15.714	15.713	0.001
0	2	1	4.32660	4.32662	-0.00003	20.511	20.511	0.000
2	1	-1	3.72743	3.72742	0.00001	23.853	23.853	0.000
2	1	1	3.43143	3.43132	0.00011	25.945	25.946	-0.001
0	4	0	2.81769	2.81769	-0.00001	31.731	31.731	0.000
2	3	-1	2.72276	2.72214	0.00063	32.868	32.876	-0.008
3	0	-2	2.37203	2.37188	0.00015	37.900	37.902	-0.002
0	0	3	2.25096	2.25086	0.00011	40.023	40.025	-0.002
3	3	1	2.17200	2.17205	-0.00005	41.544	41.543	0.001
4	2	0	2.10311	2.10309	0.00003	42.971	42.972	-0.001
0	2	3	2.09019	2.09029	-0.00010	43.250	43.248	0.002
4	0	-2	1.97476	1.97484	-0.00008	45.918	45.916	0.002
2	5	-1	1.95755	1.95775	-0.00020	46.345	46.340	0.005
4	2	1		1.95747	0.00008		46.347	-0.002
4	2	-2	1.86362	1.86371	-0.00009	48.829	48.826	0.003
5	0	-2	1.66811	1.66806	0.00005	55.004	55.006	-0.002
4	2	-3	1.61245	1.61249	-0.00003	57.073	57.072	0.001
5	2	-2	1.59946	1.59947	-0.00001	57.580	57.580	0.000
3	6	0	1.59540	1.59544	-0.00004	57.740	57.739	0.001

* NUMBER OF LINES
.- LINES INPUT = 20
.- LINES INDEXED = 20
.- LINES CALCULATED = 203
* MEAN ABSOLUTE DISCREPANCIES
<Q> =0.1422E-04
<DELTA (2-THETA)> =0.1516E-02
MAX. ERROR ACCEPTED (DEG. 2-THETA) =0.3500E-01
* FIGURES OF MERIT
1.- M(20) = 68.1
2.- F(20) = 65.0(0.0015, 203)

ANGLE RANGE SCANNED : BETA MIN=100.000 Deg. BETA MAX=105.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=105.000 Deg. BETA MAX=110.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=110.000 Deg. BETA MAX=115.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=115.000 Deg. BETA MAX=120.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=120.000 Deg. BETA MAX=125.000 Deg.
ITERATION NUMBER AT EACH DICHOTOMY LEVEL :
2747 6157 5602 2088 347 86 51

END OF SEARCH FOR MONOCLINIC SOLUTIONS

--- T O T A L CALCULATION TIME : 2.440 SEC

DICVOL91 : USEFUL REFERENCES

-
- * LOUER, D. & LOUER, M. (1972). J. APPL. CRYST. 5, 271-275.
 - * BOULTIF, A. & LOUER, D. (1991). J. APPL. CRYST. 24, 987-993.

Tableau V.2 : Fichier de sortie PDFEAPC.out graphique du programme NBS*AIDS83

```

JCPDS - ICDD  ** Edit Aids PC-90 **      Revision pc      90/02/28
                Numerical Analysis Run
                PARAMETERS as INPUT:
                IJOB = 0          INCODN = 0          IBK = 0
                IWHO = 0          IOUT = 2           IINPUT = 0
                IFRMT = 0         ITHMX = 0          ICOL = 0
                IXCD = 0          IXPD = 0           IPHKL = 0
                IDOLSQ = 2

.....
                *** MONOCLINIC ***          ***          :6/ 8/07      12:44:34
0.....1.....2.....3.....4.....5.....6.....7.
9.1124 11.2708 6.7860          95.692          CELL 1
                5E A-          ESDS 2
P2/m          10          693.51          SG-I 3
P2/m          10          693.51          SG-F 4
I          FLGS 5
T-2          .00 .00 1.00 / 1.00 .00 .00 / .00 1.00 .00          MATX
1.00: 1.00 .00 .00 / .00 1.00 .00 / .00 .00 1.00          MATX C
9.112 11.271 6.786 90.00 95.69 90.00 693.51          C-IN
6.786 9.112 11.271 90.00 90.00 95.69 693.51          34          C-RD D
9.112 11.271 6.786 90.00 95.69 90.00 .8085 .6021          C-CD E
46.050 83.036 127.031 .000 .000 -6.133          DOTM
1.5406          2          PDF1 F
                :6/ 8/07 0 0 pc 90/02/28          HIST K
A          B          C          Alpha          Beta          Gamma          VOLUME
                RECIPROCAL CELL
.11028E+00 .88725E-01 .14809E+00 89.99999 84.30799 89.99999 .144193E-02
                DIRECT CELL
9.112400 11.270800 6.786000 90.00000 95.69200 90.00000 .693513E+03
1-THETA ANGLES          THTMX = 20.0 NCCY = 2 TOLMN = .0250 TOLMX = .1000
                THEMX = 29.4 DMIN = 1.570612 LAMBDA =1.5406000
                0 CONDITIONS for NON-EXTINCTION requested
                Cycle 1
                2-Theta TOLERANCE = .20000
N H K L D calc D obs Lambda 2-é calc 2-é obs 2-é DIFF WT
1 -1 1 0 7.06494 7.06492 1.540600 12.51897 12.51900 -.00003 1.00
2 0 0 1 6.75254 6.75286 1.540600 13.10062 13.10000 .00062 1.00
3 0 2 1 4.32662 4.32660 1.540600 20.51091 20.51100 -.00009 1.00
4 2 1 1 3.43132 3.43143 1.540600 25.94591 25.94500 .00091 1.00
5 -2 3 1 2.72215 2.72277 1.540600 32.87572 32.86800 .00772 1.00
                LARGEST RESIDUAL reduced to UNIT WEIGHT .00772 for OBS 5
                STANDARD ERROR UNIT WT for OBS .00233 with DEGREES of FREEDOM 1
A B C Alpha Beta Gamma VOLUME
                RECIPROCAL CELL
.11025E+00 .88729E-01 .14808E+00 90.0000 84.2796 90.0000.144138E-02
                R C CORRECTIONS
-.33379E-04 .39418E-05-.11617E-04 .0000 -.0284 .0000*****
                DIRECT CELL
9.115610 11.270300 6.786869 90.0000 95.7204 90.0000 693.781100
                D C CORRECTIONS
.003210 -.000502 .000869 .0000 .0284 .0000 .267944
                Cycle 2
                2-Theta TOLERANCE = .05000
N H K L D calc D obs Lambda 2-é calc 2-é obs 2-é DIFF WT
1 -1 1 0 7.06611 7.06492 1.540600 12.51688 12.51900 -.00212 1.00
2 0 0 1 6.75307 6.75286 1.540600 13.09958 13.10000 -.00042 1.00
3 0 2 0 5.63515 5.63492 1.540600 15.71336 15.71400 -.00064 1.00
4 0 2 1 4.32665 4.32660 1.540600 20.51078 20.51100 -.00022 1.00
5 -2 1 1 3.72904 3.72744 1.540600 23.84258 23.85300 -.01042 1.00
6 2 1 1 3.43137 3.43143 1.540600 25.94553 25.94500 .00053 1.00
7 0 4 0 2.81757 2.81769 1.540600 31.73232 31.73100 .00132 1.00
8 -2 3 1 2.72271 2.72277 1.540600 32.86866 32.86800 .00066 1.00
                LARGEST RESIDUAL reduced to UNIT WEIGHT -.01042 for OBS 5
                STANDARD ERROR UNIT WT for OBS .00316 with DEGREES of FREEDOM 4
A B C Alpha Beta Gamma VOLUME
                RECIPROCAL CELL
.11027E+00 .88722E-01 .14809E+00 90.0000 84.3004 90.0000.144168E-02

```


R C CORRECTIONS
.21794E-04-.64962E-05 .69759E-05 .0000 .0208 .0000.299537E-06

DIRECT CELL
9.113479 11.271120 6.786303 90.0000 95.6996 90.0000 693.637000

D C CORRECTIONS
-.002131 .000826 -.000566 .0000 -.0208 .0000 -.144165

Cycle 3
2-Theta TOLERANCE = .05000

N	H	K	L	D calc	D obs	Lambda	2-é calc	2-é obs	2-é DIFF	WT
1	-1	1	0	7.06547	7.06492	1.540600	12.51802	12.51900	-.00098	1.00
2	0	0	1	6.75275	6.75286	1.540600	13.10020	13.10000	.00020	1.00
3	0	2	0	5.63556	5.63492	1.540600	15.71220	15.71400	-.00180	1.00
4	0	2	1	4.32675	4.32660	1.540600	20.51029	20.51100	-.00071	1.00
5	-2	1	1	3.72795	3.72744	1.540600	23.84966	23.85300	-.00334	1.00
6	2	1	1	3.43140	3.43143	1.540600	25.94525	25.94500	.00025	1.00
7	0	4	0	2.81778	2.81769	1.540600	31.72994	31.73100	-.00106	1.00
8	-2	3	1	2.72238	2.72277	1.540600	32.87279	32.86800	.00479	1.00
9	-3	0	2	2.37223	2.37203	1.540600	37.89664	37.90000	-.00336	1.00
10	0	0	3	2.25092	2.25097	1.540600	40.02388	40.02300	.00088	1.00
11	3	3	1	2.17214	2.17200	1.540600	41.54127	41.54400	-.00273	1.00
12	0	2	3	2.09035	2.09019	1.540600	43.24669	43.25000	-.00331	1.00
13	-4	0	2	1.97514	1.97476	1.540600	45.90868	45.91800	-.00932	1.00
14	-3	6	0	1.59552	1.59541	1.540600	57.73533	57.74000	-.00467	1.00

LARGEST RESIDUAL reduced to UNIT WEIGHT -.00932 for OBS 13
STANDARD ERROR UNIT WT for OBS .00283 with DEGREES of FREEDOM 10
A B C Alpha Beta Gamma VOLUME

RECIPROCAL CELL
.11029E+00 .88724E-01 .14809E+00 90.0000 84.3049 90.0000.144192E-02

R C CORRECTIONS
.13523E-04 .17953E-05 .26741E-05 .0000 .0046 .0000.243424E-06

DIRECT CELL
9.112288 11.270900 6.786127 90.0000 95.6951 90.0000 693.519900

D C CORRECTIONS
-.001190 -.000228 -.000176 .0000 -.0046 .0000 -.117065

Cycle 4
2-Theta TOLERANCE = .05000

N	H	K	L	D calc	D obs	Lambda	2-é calc	2-é obs	2-é DIFF	WT
1	-1	1	0	7.06488	7.06492	1.540600	12.51906	12.51900	.00006	1.00
2	0	0	1	6.75263	6.75286	1.540600	13.10044	13.10000	.00044	1.00
3	0	2	0	5.63545	5.63492	1.540600	15.71252	15.71400	-.00148	1.00
4	0	2	1	4.32667	4.32660	1.540600	20.51069	20.51100	-.00031	1.00
5	-2	1	1	3.72750	3.72744	1.540600	23.85258	23.85300	-.00042	1.00
6	2	1	1	3.43123	3.43143	1.540600	25.94661	25.94500	.00161	1.00
7	0	4	0	2.81772	2.81769	1.540600	31.73059	31.73100	-.00041	1.00
8	-2	3	1	2.72218	2.72277	1.540600	32.87527	32.86800	.00727	1.00
9	-3	0	2	2.37195	2.37203	1.540600	37.90138	37.90000	.00138	1.00
10	0	0	3	2.25088	2.25097	1.540600	40.02463	40.02300	.00163	1.00
11	3	3	1	2.17201	2.17200	1.540600	41.54374	41.54400	-.00026	1.00
12	0	2	3	2.09031	2.09019	1.540600	43.24752	43.25000	-.00248	1.00
13	-4	0	2	1.97488	1.97476	1.540600	45.91512	45.91800	-.00288	1.00
14	-5	0	2	1.66809	1.66811	1.540600	55.00473	55.00400	.00072	1.00
15	-4	2	3	1.61253	1.61246	1.540600	57.07001	57.07300	-.00299	1.00
16	-3	6	0	1.59545	1.59541	1.540600	57.73840	57.74000	-.00160	1.00

LARGEST RESIDUAL reduced to UNIT WEIGHT .00727 for OBS 8
STANDARD ERROR UNIT WT for OBS .00269 with DEGREES of FREEDOM 12
A B C Alpha Beta Gamma VOLUME

RECIPROCAL CELL
.11028E+00 .88725E-01 .14809E+00 90.0000 84.3069 90.0000.144193E-02

R C CORRECTIONS
-.18268E-05 .63270E-06 .14257E-05 .0000 .0020 .0000.535510E-08

DIRECT CELL
9.112408 11.270810 6.786037 90.0000 95.6930 90.0000 693.517300

D C CORRECTIONS
.000119 -.000081 -.000089 .0000 -.0020 .0000 -.002563

Cycle 5
2-Theta TOLERANCE = .05000

N	H	K	L	D calc	D obs	Lambda	2-é calc	2-é obs	2-é DIFF	WT
1	-1	1	0	7.06494	7.06492	1.540600	12.51897	12.51900	-.00003	1.00
2	0	0	1	6.75257	6.75286	1.540600	13.10057	13.10000	.00057	1.00
3	0	2	0	5.63541	5.63492	1.540600	15.71263	15.71400	-.00137	1.00

4	0	2	1	4.32663	4.32660	1.540600	20.51086	20.51100	-.00014	1.00
5	-2	1	1	3.72747	3.72744	1.540600	23.85279	23.85300	-.00022	1.00
6	2	1	1	3.43129	3.43143	1.540600	25.94608	25.94500	.00108	1.00
7	0	4	0	2.81770	2.81769	1.540600	31.73083	31.73100	-.00018	1.00
8	-2	3	1	2.72216	2.72277	1.540600	32.87555	32.86800	.00755	1.00
9	-3	0	2	2.37191	2.37203	1.540600	37.90194	37.90000	.00193	1.00
10	0	0	3	2.25086	2.25097	1.540600	40.02504	40.02300	.00204	1.00
11	3	3	1	2.17204	2.17200	1.540600	41.54316	41.54400	-.00084	1.00
12	0	2	3	2.09029	2.09019	1.540600	43.24795	43.25000	-.00205	1.00
13	-4	0	2	1.97486	1.97476	1.540600	45.91555	45.91800	-.00245	1.00
14	-5	0	2	1.66808	1.66811	1.540600	55.00499	55.00400	.00099	1.00
15	-4	2	3	1.61251	1.61246	1.540600	57.07096	57.07300	-.00204	1.00
16	-3	6	0	1.59544	1.59541	1.540600	57.73844	57.74000	-.00156	1.00

LARGEST RESIDUAL reduced to UNIT WEIGHT .00755 for OBS 8

STANDARD ERROR UNIT WT for OBS .00269 with DEGREES of FREEDOM 12

A	B	C	Alpha	Beta	Gamma	VOLUME
RECIPROCAL CELL						
.11028E+00	.88725E-01	.14809E+00	90.0000	84.3069	90.0000	.144192E-02
R C STNDRD ERRS						
.63321E-05	.41001E-05	.64438E-05	.0000	.0045	.0000	.0000
R C CORRECTIONS						
.44101E-08	-.55558E-08	-.14484E-07	.0000	.0000	.0000	*****
DIRECT CELL						
9.112408	11.270820	6.786038	90.0000	95.6930	90.0000	693.517500
D C STNDRD ERRS						
.000475	.000521	.000288	.0000	.0045	.0000	.041854
D C CORRECTIONS						
.000000	.000002	.000001	.0000	.0000	.0000	.000122

DIRECT CELL VARIANCE-COVARIANCE MATRIX						ROW
.225446E-06	-.999682E-07	-.425538E-07	.000000E+00	-.238173E-07	.000000E+00	1
-.999682E-07	.271280E-06	-.285651E-08	.000000E+00	.127286E-07	.000000E+00	2
-.425538E-07	-.285651E-08	.829509E-07	.000000E+00	-.107460E-08	.000000E+00	3
.000000E+00	.000000E+00	.000000E+00	.000000E+00	.000000E+00	.000000E+00	4
-.238173E-07	.127286E-07	-.107460E-08	.000000E+00	.608129E-08	.000000E+00	5
.000000E+00	.000000E+00	.000000E+00	.000000E+00	.000000E+00	.000000E+00	6

DIRECT CELL CORRELATION MATRIX						ROW
1.000000	-.404233	-.311176	.000000	-.643241	.000000	1
-.404233	1.000000	-.019042	.000000	.313382	.000000	2
-.311176	-.019042	1.000000	.000000	-.047845	.000000	3
.000000	.000000	.000000	.000000	.000000	.000000	4
-.643241	.313382	-.047845	.000000	1.000000	.000000	5
.000000	.000000	.000000	.000000	.000000	.000000	6

		<AUTHOR >	<PROGRAM>			OBS		CALC		DIFF		FINL		
N	D	calc	D obs	INT	H	K	L	H	K	L	2Theta	2Theta	2Theta	WT
		1	11.2708						0	1	0		7.838	
		2	9.0675						1	0	0		9.747	
3	7.0649	7.0649	0	-1	1	0C	-1	1	0		12.519	12.519	.000	1.0
4	6.7526	6.7529	0	0	0	1C	0	0	1		13.100	13.101	.001	1.0
		5	5.7925						0	1	1		15.284	
		6	5.6931						-1	0	1		15.552	
7	5.6354	5.6349	0	0	2	0C	0	2	0		15.714	15.713	-.001	1.0
		8	5.1754						1	0	1		17.119	
		9	5.0816						-1	1	1		17.438	
		10	4.7863						1	2	0		18.523	
		11	4.7033						1	1	1		18.853	
		12	4.5337						2	0	0		19.564	
13	4.3266	4.3266	0	0	2	1C	0	2	1		20.511	20.511	.000	1.0
		14	4.2062						2	1	0		21.105	
		15	4.0051						-1	2	1		22.178	
		16	3.9497						-2	0	1		22.493	
		17	3.8118						1	2	1		23.317	
		18	3.7569						0	3	0		23.663	
19	3.7275	3.7274	0	-2	1	1C	-2	1	1		23.853	23.853	.000	1.0
		20	3.6023						2	0	1		24.695	
		21	3.5325						-2	2	0		25.191	
		22	3.4708						1	3	0		25.646	
23	3.4313	3.4314	0	2	1	1C	2	1	1		25.945	25.946	.001	1.0
		24	3.3763						0	0	2		26.376	
		25	3.2830						0	3	1		27.140	
		26	3.2720						-1	0	2		27.233	

