

## Lampiran 4

### 4.1 Input Rietveld

#### A. Perbandingan $\text{ZrO}_2\text{-CuO}$ 1 : 1

```
ZrO2-CuO
  0  4  2  0  0  0  0  0  0  1  0  0
0011100002050000000  0.000  0.000 0.00000
  1.5406 1.54439 0.50000  1.00  7.0000  1.0000  0.00 20.0000  0.0000  0.000
 300.100.900.900.90 10.025  0.017 99.980  0.000  0.000
      7
  0.000  0.000
-0.525286 11.000
  81.290000  0.0000E+0  0.0000E+0  0.0000E+0  0.0000E+0  0.0000E+0
  21.000  0.000  0.000  0.000  0.000  0.000
ZrO2
  3  1  0.0 0.0 1.0  0.0 0.0 1.0
P 2/C
ZR  ZR  0.27580 0.04110 0.20820 1.00000 1.00000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O  O  0.07030 0.33590 0.34060 1.00000 1.00000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O  O  0.44230 0.75490 0.47890 0.50000 1.00000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
-2.535910E-06  0.0000
-0.84000 0.87000 0.02000 0.00000
  5.1450  5.2070  5.3110 90.0000 99.2000 90.0000
  1.00000 0.00000 0.02000 0.00000
  0.20000 0.00000 0.00000 0.00000
  0.000  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000  0.000  0.000
 31.000  0.000
 41.000 51.000  0.000  0.000
  0.000  0.000  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000
CuO
  2  1  0.0 0.0 1.0  0.0 0.0 1.0
C 2/C
CU  CU  0.25000 0.25000 0.00000 1.00000 0.50000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O  O  0.00000 0.41840 0.25000 1.00000 0.50000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
1.792610E-04  0.0000
  0.87000-0.00500 0.02000 0.00000
  4.6837  3.4226  5.1288 90.0000 99.5400 90.0000
  1.00000 0.00000 0.02000 0.00000
  0.20000 0.00000 0.00000 0.00000
  0.000  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000  0.000  0.000
 61.000  0.000
 71.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000
  0.000  0.000  0.000  0.000
```

#### B. Perbandingan $\text{ZrO}_2\text{-CuO}$ 1 : 8

```

ZrCuO
  0   4   2   0   0   0   0   0   0   0   0   0
0011100002050000000  0.000  0.000 0.00000
  1.5406 1.54439 0.50000  1.00  7.0000  1.0000  0.00 20.0000  0.0000  0.000
  300.100.900.900.900.90 20.050  0.033  99.980  0.000  0.000
    29
    0.000  0.000
    388.600000  0.0000E+0  0.0000E+0  0.0000E+0  0.0000E+0  0.0000E+0
    11.000  0.000  0.000  0.000  0.000  0.000  0.000
ZrO2
  3   1   0.0 0.0 1.0  0.0 0.0 1.0
P 21/C
ZR  ZR  0.27582 0.04112 0.20822 1.00000 0.25000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O   O   0.07032 0.33591 0.34061 0.00000 0.50000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O   O   0.44232 0.75491 0.47891 1.00000 0.25000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
5.134780E-03  2.6562
-3.00000 2.70000-0.35000 0.00000
  5.1807  5.1494  5.2785 89.9866 99.6537 89.9997
  1.00000 0.00000 0.02000 0.00000
  4.66390-0.14689 0.00124 0.00000
    0.000  0.000  0.000  0.000  0.000
    0.000  0.000  0.000  0.000  0.000  0.000
    0.000  0.000  0.000  0.000  0.000
    0.000  0.000  0.000  0.000  0.000  0.000
    0.000  0.000  0.000  0.000  0.000  0.000
    0.000  0.000  0.000  0.000  0.000  0.000
    21.000  31.000
    41.000  51.000  61.000  0.000
    71.000  81.000  91.000 101.000 111.000 121.000
    0.000  0.000  0.000  0.000
    131.000 141.000 151.000  0.000
CuO
  2   1   0.0 0.0 1.0  0.0 0.0 1.0
C 2/C
CU  CU  0.25000 0.25000 0.00000 0.80000 0.50000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
O   O   0.00000 0.41840 0.25000 0.70000 0.50000
  0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
1.785330E-03  0.3876
  2.50000-2.00000 0.43000 0.00000
  4.6807  3.4222  5.1289 90.0281 99.3975 89.9670
  1.00000 0.00000 0.02000 0.00000
-2.79280 0.14591-0.00150 0.00000
    0.000  0.000  0.000  0.000  0.000
    0.000  0.000  0.000  0.000  0.000  0.000
    0.000  0.000  0.000  0.000  0.000
    0.000  0.000  0.000  0.000  0.000  0.000
    161.000  171.000
    181.000 191.000 201.000  0.000
    211.000 221.000 231.000 241.000 251.000 261.000
    0.000  0.000  0.000  0.000
    271.000 281.000 291.000  0.000

```

## 4.2 Output Rietveld

### A. Perbandingan ZrO<sub>2</sub>-CuO 1 : 1

```

**** MULTI-RIETVELD ANALYSIS PROGRAM LH-RIET 6.800
ZrO2-CuO
NUMBER OF PHASES =      2
NUMBER OF HISTOGRAMS =    1
NUMBER OF PARAMETER LIMITS =    0

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NUMBER OF BOND RESTRAINTS = 0

\*\*\* HISTOGRAM 1 \*\*\*

FOR X-RAY DATA  
NEWTON-RAPHSON ALGORITHM  
BACKGROUND TO BE REFINED (MAX 6 PARAMETERS)  
- POLYNOMIAL BACKGROUND  
THE PSEDUO-VOIGT PROFILE FUNCTION WAS SELECTED  
- USING THE HOWARD, SUM OF 5 PEAKS, ASYMMETRY  
WAVELENGTHS = 1.54060 1.54439  
ALPHA2:ALPHA1 RATIO = .5000  
BASE OF PEAK = 2.0\*HW\* 7.00  
MONOCHROMATOR CORRECTION = 1.0000  
ABSORPTION CORRECTION FOR CYLINDER SAMPLE  
USING ALGORITHM OF SABINE(1996)/DWIGGINS(1972) WITH mu = .0000  
NO ILLUMINATION CORRECTION  
PREFERRED ORIENTATION USING MARCH MODEL - NO SUMMING OF EQUIVALENTS  
HISTOGRAM WEIGHTING = 1.0000  
USING BRAGG-BRENTANO SAMPLE DISPLACEMENT

GENERATE OFF-LINE PLOT

- ILL PLOT FILE OF OBS AND CALC DATA

OUTPUT STRUCTURE FACTORS

OUTPUT CORRELATION MATRIX

GENERATE NEW INPUT FILE

NUMBER OF CYCLES = 30

RELAXATION FACTORS:

FOR COORDINATES, ISOTROPIC B, SITE OCCUPANCY = .90

FOR ANISOTROPIC TEMPERATURE FACTORS = .90

FOR SCALE, ZERO, B OVERALL, UNIT CELL, PREFERRED ORIENTATION BACKGROUND = .90

FOR PEAK WIDTH, ASYMMETRY, SHAPE PARAMETERS = .90

EPS-VALUE = .100

NUMBER OF PARAMETERS VARIED = 7

GLOBAL PARAMETERS AND CODEWORDS:

ZEROPOINT( 1) = .00 .00

SAMPLE DISPLACEMENT( 1) = -.52537 11.00

HISTOGRAM READ IN AS (2THETA, INTENSITY)

HISTOGRAM 1 FROM 10.025400 TO 99.980000 IN STEPS OF .017000 DEGREES

BACKGROUND PARAMETERS AND CODEWORDS( 1)

81.280000	.000000	.000000	.000000	.000000	.000000	.000000
21.000000	.000000	.000000	.000000	.000000	.000000	.000000

\*\*\*\*\* PHASE 1 \*\*\*\*\*

ZrO2

PHASE IS CALCULATED USING STRUCTURAL INPUT

NUMBER OF FORMULA PER UNIT CELL = 1

NUMBER OF ATOMS = 3

PREFERRED ORIENTATION VECTOR( 1) = .0000 .0000 1.0000

THE SPACE GROUP IS P 2/C

\*\*\*INITIAL PARAMETERS\*\*\*

ATOM	NTYP	X	Y	Z	B	N	
		B11	B22	B33	B12	B13	B23
ZR	ZR	.27580	.04110	.20820	1.00000	1.00000	
		.00000	.00000	.00000	.00000	.00000	.00000
O	O	.07030	.33590	.34060	1.00000	1.00000	
		.00000	.00000	.00000	.00000	.00000	.00000
O	O	.44230	.75490	.47890	.50000	1.00000	
		.00000	.00000	.00000	.00000	.00000	.00000

\*\*\*\*\* PHASE INFORMATION \*\*\*\*\*

OVERALL SCALE FACTOR = -2.55150

OVERALL TEMP. FACTOR = .00000

DIRECT CELL PARAMETERS = 5.1450 5.2070 5.3110 90.0000 99.2000 90.0000

\*\*\* HISTOGRAM 1 \*\*\*

HISTOGRAM SCALE FACTOR = 1.00000 .00

PREFERRED ORIENTATION PARAMETER = 1.0000

ABSORPTION R = .0000

ASYMMETRY PARAMETERS = .020000 .000000

GAUSSIAN HALF-WIDTH PARAMETERS = -.8400 .8700 .0200

ANISOTROPIC PARAMETER = .000000

PSEUDO-VOIGT PEAK SHAPE =

.2000 + .00000 \* TWOTH + .000000 \* TWOTHSQ

EXTINCTION PARAMETER = .000000

The Laue symmetry is: 2/M

\*\*\*CODING OF VARIABLES\*\*\*

ATOM	X B11	Y B22	Z B33	B B12	N B13	B23
ZR	.00	.00	.00	.00	.00	
	.00	.00	.00	.00	.00	.00
O	.00	.00	.00	.00	.00	
	.00	.00	.00	.00	.00	.00
O	.00	.00	.00	.00	.00	
	.00	.00	.00	.00	.00	.00

\*\*\*\*\* PHASE INFORMATION CODEWORDS \*\*\*\*\*

OVERALL SCALE FACTOR = 31.00

OVERALL TEMP. FACTOR = .00

CELL CONSTANTS = .00 .00 .00 .00 .00 .00

\*\*\* HISTOGRAM 1 CODEWORDS \*\*\*

PREFERRED ORIENTATION PARAMETER = .00

ABSORPTION R/Po PARAMETER = .00

ASYMMETRY PARAMETERS = .00 .00

GAUSSIAN COMPONENT = 41.00 51.00 .00

ANISOTROPIC = .00

LORENZTIAN COMPONENTS = .00 .00 .00

EXTINCTION = .00

FORMFACTORS FOR HISTOGRAM

FOR ZR DFP= -.314000 DFPP= 2.245000

COEFFICIENTS= 17.876500 1.276180 10.948000 11.916000 5.417320 .117622 3.657210  
87.662700 2.069290

FOR O DFP= .047000 DFPP= .032000

COEFFICIENTS= 3.048500 13.277100 2.286800 5.701100 1.546300 .323900 .867000  
32.908900 .250800

LAUE SYMMETRY 2/M WILL BE USED TO GENERATE INDICES

\*\*\*\*\* PHASE 2 \*\*\*\*\*

CuO

PHASE IS CALCULATED USING STRUCTURAL INPUT

NUMBER OF FORMULA PER UNIT CELL = 1

NUMBER OF ATOMS = 2

PREFERRED ORIENTATION VECTOR( 1) = .0000 .0000 1.0000

THE SPACE GROUP IS C 2/C

\*\*\*INITIAL PARAMETERS\*\*\*

ATOM	NTYP	X B11	Y B22	Z B33	B B12	N B13	B23
CU	CU	.25000	.25000	.00000	1.00000	.50000	
		.00000	.00000	.00000	.00000	.00000	.00000
O	O	.00000	.41840	.25000	1.00000	.50000	
		.00000	.00000	.00000	.00000	.00000	.00000

\*\*\*\*\* PHASE INFORMATION \*\*\*\*\*

OVERALL SCALE FACTOR = .179141E-03

OVERALL TEMP. FACTOR = .00000

DIRECT CELL PARAMETERS = 4.6837 3.4226 5.1288 90.0000 99.5400 90.0000



ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								

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+-----+
|               Phase: 1               |
+-----+

```

```

PHASE SCALE FACTOR   = -.255151      2.29635      .366634E-01
OVERALL TEMP. FACTOR =   .000000      .000000      .000000
CELL PARAMETERS      =   5.145000      .000000      .000000
                      =   5.207000      .000000      .000000
                      =   5.311000      .000000      .000000
                      =  90.000010      .000008      .000000
                      =  99.200000      .000008      .000000
                      =  90.000010      .000008      .000000
RECIPROCAL CELL      =   .197      .192      .191      90.000      80.800      90.000
CELL VOLUME          =  140.451500      .000000
SCALE * VOLUME       =  -35.836340      5.149429
MOLECULAR WEIGHT     =   492.880
DENSITY              =    5.825

```

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM<sup>2</sup> ( in cm<sup>-2</sup>)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = -.118534E+08

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+-----+
|               Histogram: 1               |
+-----+

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```

SCALE FACTOR          = 1.0000      .000000      .000000
ZEROPOINT             =   .000000      .000000      .000000

SAMPLE DISPLACEMENT  =   -.52537      .000000      .00147

BACKGROUND PARAMETER B 0 =   80.3191      -.960876      12398.6
PREFERRED ORIENTATION =   1.00000      .000000      .000000
ABSORPTION R          =   .00000      .000000      .000000
ASYMMETRY PARAMETERS  =   .02000      .000000      .000000
                      =   .00000      .000000      .000000
HALFWIDTH PARAMETERS U =   -.840000      .000000      .000782
                      V =   .870000      .000000      .000865
                      W =   .020000      .000000      .000000
ANISOTROPIC GAUSSIAN BROADENING =   .000000      .000000      .000000
PEAK SHAPE PARAMETER Gam0 =   .200000      .000000      .000000
PEAK SHAPE PARAMETER Gam1 =   .000000      .000000      .000000
PEAK SHAPE PARAMETER Gam2 =   .000000      .000000      .000000
EXTINCTION PARAMETER  =   .000000      .000000      .000000

```

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					

O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000
1.0000	.0000	.0000	.5000	.0000	.0000				
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33	
SB33									
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23	
SB23									
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									

```

+-----+
|                               |
|           Phase:  2         |
|                               |
+-----+

```

PHASE SCALE FACTOR	=	.183352E-03	.421093E-05	.246340	
OVERALL TEMP. FACTOR	=	.000000	.000000	.000000	
CELL PARAMETERS	=	4.683700	.000000	.000000	
		3.422600	.000000	.000000	
		5.128799	.000000	.000000	
		90.000010	.000008	.000000	
		99.540010	.000008	.000000	
		90.000010	.000008	.000000	
RECIPROCAL CELL	=	.217	.292	.198	90.000 80.460 90.000
CELL VOLUME	=	81.079820	.000000		
SCALE * VOLUME	=	.014866	19.973210		
MOLECULAR WEIGHT	=	318.200			
DENSITY	=	6.514			

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = 3174.51

```

+-----+
|                               |
|           Histogram: 1       |
|                               |
+-----+

```

SCALE FACTOR	=	1.0000	.00000	.00000	
ZEROPOINT	=	.00000	.00000	.00000	
SAMPLE DISPLACEMENT	=	-.52537	.00000	.00147	
BACKGROUND PARAMETER B 0	=	80.3191	-.960876		12398.6
PREFERRED ORIENTATION	=	1.00000	.00000	.00000	
ABSORPTION R	=	.00000	.00000	.00000	
ASYMMETRY PARAMETERS	=	.02000	.00000	.00000	
		.00000	.00000	.00000	
HALFWIDTH PARAMETERS U	=	.904432	.034432		3932.730000
	V	-.005000	.000000		.000000
	W	.020000	.000000		.000000
ANISOTROPIC GAUSSIAN BROADENING	=	.000000	.000000		.000000
PEAK SHAPE PARAMETER Gam0	=	.200000	.000000	.000000	
PEAK SHAPE PARAMETER Gam1	=	.000000	.000000	.000000	
PEAK SHAPE PARAMETER Gam2	=	.000000	.000000	.000000	
EXTINCTION PARAMETER	=	.000000	.000000	.000000	

MOLAR PERCENTAGE OF PHASES:

PHASE 1: \*\*\*\*\*  
 PHASE 2: 1.49 \*\*\*\*\*

WEIGHT PERCENTAGE OF PHASES:

100.03 -41.34  
 -.03 -35.99

```

+-----+
| Hist |  Rp  |  Rwp  |  Rexp |Durbin Unwght| Durbin Wght |  N-P  |
+-----+

```

1	*****	*****	10.78	.026	.025	5285
SUMYDIF	SUMYOBS	SUMYCALC	SUMWYOBSSQ	GOF	CONDITION	
.1206E+10	.4546E+06	-.1205E+10	.4546E+06	.8621E+10	.5006E+18	

+++++

CYCLE NUMBER= 2

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
ZR	.27580	.00000	.00000	.04110	.00000	.00000	.20820	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.07030	.00000	.00000	.33590	.00000	.00000	.34060	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.44230	.00000	.00000	.75490	.00000	.00000	.47890	.00000	.00000	
.5000	.0000	.0000	1.0000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

Phase: 1

PHASE SCALE FACTOR = -.255176E-01 .229633 .366683E-02  
OVERALL TEMP. FACTOR = .000000 .000000 .000000  
CELL PARAMETERS = 5.145000 .000000 .000000  
5.207000 .000000 .000000  
5.311000 .000000 .000000  
90.000010 .000000 .000000  
99.200000 .000000 .000000  
90.000010 .000000 .000000  
RECIPROCAL CELL = .197 .192 .191 90.000 80.800 90.000  
CELL VOLUME = 140.451500 .000000  
SCALE \* VOLUME = -3.583985 .515011  
MOLECULAR WEIGHT = 492.880  
DENSITY = 5.825

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = -.118546E+07

Histogram: 1



```

SCALE FACTOR          = 1.0000    .00000    .00000
ZEROPOINT             =      .00000    .00000    .00000
SAMPLE DISPLACEMENT   =     - .52537    .00000    .00147

BACKGROUND PARAMETER B 0 =      81.1262      .807084      1240.26
PREFERRED ORIENTATION   =      1.00000    .00000    .00000
ABSORPTION R           =      .00000    .00000    .00000
ASYMMETRY PARAMETERS    =      .02000    .00000    .00000
                        .00000    .00000    .00000
HALFWIDTH PARAMETERS U  =      -.840000    .000000      .000782
                        V      =      .870000    .000000      .000866
                        W      =      .020000    .000000      .000000
ANISOTROPIC GAUSSIAN BROADENING =      .000000    .000000      .000000
PEAK SHAPE PARAMETER Gam0 =      .200000    .000000    .000000
PEAK SHAPE PARAMETER Gam1 =      .000000    .000000    .000000
PEAK SHAPE PARAMETER Gam2 =      .000000    .000000    .000000
EXTINCTION PARAMETER    =      .000000    .000000    .000000

```

PHASE 2: CuO  
NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	.00000
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	.00000
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33	SB33	
ATOM	B12	DB12	SB12	B13	DB13	SB13	B23	DB23	SB23	
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000

```

+-----+
|                               |
|                               |
+-----+
PHASE SCALE FACTOR  = .180312E-03-.304007E-05 .247401E-01
OVERALL TEMP. FACTOR = .000000 .000000 .000000
CELL PARAMETERS     =  4.683700 .000000 .000000
                    3.422600 .000000 .000000
                    5.128799 .000000 .000000
                    90.000010 .000000 .000000
                    99.540010 .000000 .000000
                    90.000010 .000000 .000000
RECIPROCAL CELL     = .217 .292 .198 90.000 80.460 90.000
CELL VOLUME         = 81.079820 .000000
SCALE * VOLUME      = .014620 2.005921
MOLECULAR WEIGHT     = 318.200
DENSITY             = 6.514
ABSOLUTE PHASE VALUES:
  INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
  MASS = MASS OF PHASE IN BEAM (in g)
  ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR
Then:
  INC*MASS*ls/R = 3121.87

```

```

+-----+
|                               |
|                               |
+-----+

```

```

SCALE FACTOR          = 1.0000    .00000    .00000
ZEROPOINT             =      .00000    .00000    .00000
SAMPLE DISPLACEMENT   =     - .52537    .00000    .00147

BACKGROUND PARAMETER B 0 =      81.1262      .807084      1240.26
PREFERRED ORIENTATION   =      1.00000    .00000    .00000
ABSORPTION R           =      .00000    .00000    .00000
ASYMMETRY PARAMETERS    =      .02000    .00000    .00000
                        .00000    .00000    .00000
HALFWIDTH PARAMETERS U =      .887266      -.017166      396.630600
                        V =      -.005000      .000000      .000000
                        W =      .020000      .000000      .000000
ANISOTROPIC GAUSSIAN BROADENING =      .000000      .000000      .000000
PEAK SHAPE PARAMETER Gam0 =      .200000    .000000    .000000
PEAK SHAPE PARAMETER Gam1 =      .000000    .000000    .000000
PEAK SHAPE PARAMETER Gam2 =      .000000    .000000    .000000
EXTINCTION PARAMETER    =      .000000    .000000    .000000

```

```

MOLAR PERCENTAGE OF PHASES:      WEIGHT PERCENTAGE OF PHASES:
PHASE 1:  *****  744.02          100.26  -41.66
PHASE 2:    1.46  200.61           - .26  -36.23

```

```

+-----+
| Hist |  Rp  |  Rwp  |  Rexp |Durbin Unwght| Durbin Wght |  N-P  |
+-----+
|    1  |*****|*****|  10.78 |    .026  |    .025  |  5285  |
+-----+
| SUMYDIF | SUMYOBS | SUMYCALC | SUMWYOBSQ |  GOF  | CONDITION |
+-----+
| .1206E+09| .4546E+06| -.1201E+09| .4546E+06| .8621E+08| .5012E+16|
+-----+

```

```

+++++
+++++

```

CYCLE NUMBER= 3

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
ZR	.27580	.00000	.00000	.04110	.00000	.00000	.20820	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.07030	.00000	.00000	.33590	.00000	.00000	.34060	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.44230	.00000	.00000	.75490	.00000	.00000	.47890	.00000	.00000	
.5000	.0000	.0000	1.0000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

```

+-----+

```

```

|          Phase: 1          |
+-----+-----+-----+
PHASE SCALE FACTOR   = -.255409E-02 .229635E-01 .366662E-03
OVERALL TEMP. FACTOR =   .000000   .000000   .000000
CELL PARAMETERS      =    5.145000    .000000    .000000
                        5.207000    .000000    .000000
                        5.311000    .000000    .000000
                        90.000010    .000000    .000000
                        99.200000    .000000    .000000
                        90.000010    .000000    .000000
RECIPROCAL CELL      =   .197   .192   .191  90.000  80.800  90.000
CELL VOLUME          =  140.451500  .000000
SCALE * VOLUME       =   -3.58726   .051498
MOLECULAR WEIGHT     =    492.880
DENSITY              =     5.825
ABSOLUTE PHASE VALUES:
    INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
    MASS = MASS OF PHASE IN BEAM (in g)
    ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR
Then:
    INC*MASS*ls/R = -118654.

```

PHASE 2: CuO  
NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

```

+-----+
|                               |
|                               |
+-----+
PHASE SCALE FACTOR   = .179445E-03-.866719E-06 .246878E-02
OVERALL TEMP. FACTOR = .000000 .000000 .000000
CELL PARAMETERS      = 4.683700 .000000 .000000
                     3.422600 .000000 .000000
                     5.128799 .000000 .000000
                     90.000010 .000000 .000000
                     99.540010 .000000 .000000
                     90.000010 .000000 .000000
RECIPROCAL CELL      = .217 .292 .198 90.000 80.460 90.000
CELL VOLUME          = 81.079820 .000000
SCALE * VOLUME       = .014549 .200168
MOLECULAR WEIGHT     = 318.200
DENSITY              = 6.514
ABSOLUTE PHASE VALUES:
  INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
  MASS = MASS OF PHASE IN BEAM (in g)
  ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR
Then:
  INC*MASS*ls/R = 3106.87

```

```

+-----+
|                               |
|                               |
+-----+
SCALE FACTOR          = 1.0000 .00000 .00000
ZEROPOINT             = .00000 .00000 .00000

SAMPLE DISPLACEMENT  = -.52537 .00000 .00147

BACKGROUND PARAMETER B 0 = 81.2729 .146742 124.007
PREFERRED ORIENTATION  = 1.00000 .00000 .00000
ABSORPTION R          = .00000 .00000 .00000
ASYMMETRY PARAMETERS  = .02000 .00000 .00000
                     .00000 .00000 .00000
HALFWIDTH PARAMETERS U = .877564 -.009702 39.703830
                     V = -.005000 .000000 .000000
                     W = .020000 .000000 .000000
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000
EXTINCTION PARAMETER  = .000000 .000000 .000000

MOLAR PERCENTAGE OF PHASES:      WEIGHT PERCENTAGE OF PHASES:
PHASE 1:  -35.87  9.03          102.69 -43.47
PHASE 2:   1.45 20.02           -2.69 -37.01

```

```

+-----+
| Hist | Rp | Rwp | Rexp | Durbin Unwght | Durbin Wght | N-P |
+-----+
| 1 | 2655.26 | ***** | 10.78 | .026 | .025 | 5285 |
+-----+
| SUMYDIF | SUMYOBS | SUMYCALC | SUMWYOBSQ | GOF | CONDITION |
+-----+
| .1207E+08 | .4546E+06 | -.1161E+08 | .4546E+06 | .8622E+06 | .5016E+14 |
+-----+

```

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++++
++++

```

```

CYCLE NUMBER= 4
PHASE 1: ZrO2
NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

```

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
ZR	.27580	.00000	.00000	.04110	.00000	.00000	.20820	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.07030	.00000	.00000	.33590	.00000	.00000	.34060	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.44230	.00000	.00000	.75490	.00000	.00000	.47890	.00000	.00000	
.5000	.0000	.0000	1.0000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

```

+-----+
|                               |
|                               |
+-----+

```

```

PHASE SCALE FACTOR   = -.257695E-03 .229640E-02 .366692E-04
OVERALL TEMP. FACTOR = .000000 .000000 .000000
CELL PARAMETERS      =  5.145000 .000000 .000000
                      =  5.207000 .000000 .000000
                      =  5.311000 .000000 .000000
                      = 90.000010 .000000 .000000
                      = 99.200000 .000000 .000000
                      = 90.000010 .000000 .000000
RECIPROCAL CELL      =  .197 .192 .191 90.000 80.800 90.000
CELL VOLUME          = 140.451500 .000000
SCALE * VOLUME       =  -.036194 .005150
MOLECULAR WEIGHT     =  492.880
DENSITY              =  5.825

```

#### ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM<sup>2</sup> ( in cm<sup>-2</sup>)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = -11971.6

```

+-----+
|                               |
|                               |
+-----+

```

```

SCALE FACTOR          = 1.0000 .00000 .00000
ZEROPOINT             = .00000 .00000 .00000

SAMPLE DISPLACEMENT  =  -.52537 .00000 .00147

BACKGROUND PARAMETER B 0 =  81.2849 .119772E-01 12.4011
PREFERRED ORIENTATION =  1.00000 .00000 .00000
ABSORPTION R          =  .00000 .00000 .00000
ASYMMETRY PARAMETERS  =  .02000 .00000 .00000
                      =  .00000 .00000 .00000

HALFWIDTH PARAMETERS U =  -.839999 .000000 .000781
                      V =  .869999 -.000001 .000864
                      W =  .020000 .000000 .000000

ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000

```

PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000  
EXTINCTION PARAMETER = .000000 .000000 .000000  
PHASE 2: CuO  
NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

+-----+  
| Phase: 2 |  
+-----+

PHASE SCALE FACTOR = .179301E-03-.144212E-06 .246607E-03  
OVERALL TEMP. FACTOR = .000000 .000000 .000000  
CELL PARAMETERS = 4.683700 .000000 .000000  
3.422600 .000000 .000000  
5.128799 .000000 .000000  
90.000010 .000000 .000000  
99.540010 .000000 .000000  
90.000010 .000000 .000000  
RECIPROCAL CELL = .217 .292 .198 90.000 80.460 90.000  
CELL VOLUME = 81.079820 .000000  
SCALE \* VOLUME = .014538 .019995  
MOLECULAR WEIGHT = 318.200  
DENSITY = 6.514

#### ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM<sup>2</sup> ( in cm<sup>-2</sup>)  
MASS = MASS OF PHASE IN BEAM (in g)  
ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = 3104.37

+-----+  
| Histogram: 1 |  
+-----+

SCALE FACTOR = 1.0000 .00000 .00000  
ZEROPOINT = .00000 .00000 .00000  
SAMPLE DISPLACEMENT = -.52537 .00000 .00147  
BACKGROUND PARAMETER B 0 = 81.2849 .119772E-01 12.4011  
PREFERRED ORIENTATION = 1.00000 .00000 .00000  
ABSORPTION R = .00000 .00000 .00000  
ASYMMETRY PARAMETERS = .02000 .00000 .00000  
.00000 .00000 .00000  
HALFWIDTH PARAMETERS U = .875155 -.002409 3.954371  
V = -.005000 .000000 .000000  
W = .020000 .000000 .000000  
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000  
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000  
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000  
PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000

EXTINCTION PARAMETER = .000000 .000000 .000000

MOLAR PERCENTAGE OF PHASES: WEIGHT PERCENTAGE OF PHASES:  
PHASE 1: -3.62 .52 135.01 -72.58  
PHASE 2: 1.45 2.00 -35.01 -51.46

```
+-----+
| Hist | Rp | Rwp | Rexp | Durbin Unwght | Durbin Wght | N-P |
+-----+
| 1 | 269.04 | 1001.23 | 10.78 | .026 | .024 | 5285 |
+-----+
| SUMYDIF | SUMYOBS | SUMYCALC | SUMWYOBSQ | GOF | CONDITION |
+-----+
| .1223E+07 | .4546E+06 | -.7609E+06 | .4546E+06 | .8624E+04 | .5075E+12 |
+-----+
```

+++++

CYCLE NUMBER= 5

PHASE 1: ZrO2  
NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
ZR	.27580	.00000	.00000	.04110	.00000	.00000	.20820	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.07030	.00000	.00000	.33590	.00000	.00000	.34060	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.44230	.00000	.00000	.75490	.00000	.00000	.47890	.00000	.00000	
.5000	.0000	.0000	1.0000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

```
+-----+
| Phase: 1 |
+-----+
```

PHASE SCALE FACTOR = -.280467E-04 .229648E-03 .370474E-05  
OVERALL TEMP. FACTOR = .000000 .000000 .000000  
CELL PARAMETERS = 5.145000 .000000 .000000  
5.207000 .000000 .000000  
5.311000 .000000 .000000  
90.000010 .000000 .000000  
99.200000 .000000 .000000  
90.000010 .000000 .000000  
RECIPROCAL CELL = .197 .192 .191 90.000 80.800 90.000  
CELL VOLUME = 140.451500 .000000  
SCALE \* VOLUME = -.003939 .000520  
MOLECULAR WEIGHT = 492.880  
DENSITY = 5.825  
ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)  
 MASS = MASS OF PHASE IN BEAM (in g)  
 ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR  
 Then:  
 INC\*MASS\*ls/R = -1302.95

```

+-----+
|                               |
|           Histogram: 1       |
|                               |
+-----+
SCALE FACTOR          = 1.0000 .00000 .00000
ZEROPOINT             = .00000 .00000 .00000

SAMPLE DISPLACEMENT   = -.52541 -.00004 .00147

BACKGROUND PARAMETER B 0 = 81.2858 .877452E-03 1.25287
PREFERRED ORIENTATION  = 1.00000 .00000 .00000
ABSORPTION R           = .00000 .00000 .00000
ASYMMETRY PARAMETERS   = .02000 .00000 .00000
                        .00000 .00000 .00000
HALFWIDTH PARAMETERS U = -.839995 .000005 .000783
                        V = .869991 -.000008 .000866
                        W = .020000 .000000 .000000
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000
EXTINCTION PARAMETER    = .000000 .000000 .000000
  
```

PHASE 2: CuO  
 NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

```

+-----+
|                               |
|           Phase: 2           |
|                               |
+-----+
PHASE SCALE FACTOR    = .179266E-03-.353188E-07 .249075E-04
OVERALL TEMP. FACTOR  = .000000 .000000 .000000
CELL PARAMETERS       = 4.683700 .000000 .000000
                        3.422600 .000000 .000000
                        5.128799 .000000 .000000
                        90.000010 .000000 .000000
                        99.540010 .000000 .000000
                        90.000010 .000000 .000000
RECIPROCAL CELL       = .217 .292 .198 90.000 80.460 90.000
CELL VOLUME           = 81.079820 .000000
SCALE * VOLUME        = .014535 .002019
MOLECULAR WEIGHT      = 318.200
DENSITY               = 6.514
  
```



```

ABSOLUTE PHASE VALUES:
  INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
  MASS = MASS OF PHASE IN BEAM (in g)
  ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR
Then:
  INC*MASS*ls/R = 3103.76

```

MOLAR PERCENTAGE OF PHASES:			WEIGHT PERCENTAGE OF PHASES:	
PHASE 1:	-37.18	8.81	-72.35	20.96
PHASE 2:	137.18	33.05	172.35	50.48

Hist	Rp	Rwp	Rexp	Durbin Unwght	Durbin Wght	N-P
1	33.38	101.16	10.78	.044	.037	5285
SUMYDIF	SUMYOBS	SUMYCALC	SUMWYOBSQ	GOF	CONDITION	
.1518E+06	.4546E+06	.3245E+06	.4546E+06	.8802E+02	.1332E+12	

```

+++++
+++++

```

CYCLE NUMBER= 6

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

[illegible]

```

.000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
O .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
.000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
O .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
.000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000

```

```

+-----+
|                               |
|                               |
+-----+

```

```

PHASE SCALE FACTOR = -.508244E-05 .229642E-04 .645408E-06
OVERALL TEMP. FACTOR = .000000 .000000 .000000
CELL PARAMETERS = 5.145000 .000000 .000000
                    5.207000 .000000 .000000
                    5.311000 .000000 .000000
                    90.000010 .000000 .000000
                    99.200000 .000000 .000000
                    90.000010 .000000 .000000
RECIPROCAL CELL = .197 .192 .191 90.000 80.800 90.000
CELL VOLUME = 140.451500 .000000
SCALE * VOLUME = -.000714 .000091
MOLECULAR WEIGHT = 492.880
DENSITY = 5.825

```

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM<sup>2</sup> ( in cm<sup>-2</sup>)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = -236.112

```

+-----+
|                               |
|                               |
+-----+

```

```

SCALE FACTOR = 1.0000 .00000 .00000
ZEROPOINT = .00000 .00000 .00000

SAMPLE DISPLACEMENT = -.52573 -.00031 .00229

BACKGROUND PARAMETER B 0 = 81.2861 .253348E-03 .218243
PREFERRED ORIENTATION = 1.00000 .00000 .00000
ABSORPTION R = .00000 .00000 .00000
ASYMMETRY PARAMETERS = .02000 .00000 .00000
                    .00000 .00000 .00000
HALFWIDTH PARAMETERS U = -.839959 .000036 .001254
                        V = .869923 -.000067 .001387
                        W = .020000 .000000 .000000
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000
EXTINCTION PARAMETER = .000000 .000000 .000000

```

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					

ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33
SB33								
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23
SB23								
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000

```

+-----+
|                               |
|           Phase:  2         |
|                               |
+-----+

```

```

PHASE SCALE FACTOR   = .179259E-03-.679658E-08 .433841E-05
OVERALL TEMP. FACTOR = .000000 .000000 .000000
CELL PARAMETERS      =  4.683700 .000000 .000000
                      3.422600 .000000 .000000
                      5.128799 .000000 .000000
                      90.000010 .000000 .000000
                      99.540010 .000000 .000000
                      90.000010 .000000 .000000
RECIPROCAL CELL      =  .217 .292 .198 90.000 80.460 90.000
CELL VOLUME          =  81.079820 .000000
SCALE * VOLUME       =  .014534 .000352
MOLECULAR WEIGHT     =  318.200
DENSITY              =  6.514

```

ABSOLUTE PHASE VALUES:

```

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
MASS = MASS OF PHASE IN BEAM (in g)
ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

```

Then:

INC\*MASS\*ls/R = 3103.64

```

+-----+
|                               |
|           Histogram:  1         |
|                               |
+-----+

```

```

SCALE FACTOR          = 1.0000 .00000 .00000
ZEROPOINT             = .00000 .00000 .00000

SAMPLE DISPLACEMENT  = -.52573 -.00031 .00229

BACKGROUND PARAMETER B 0 = 81.2861 .253348E-03 .218243
PREFERRED ORIENTATION  = 1.00000 .00000 .00000
ABSORPTION R          = .00000 .00000 .00000
ASYMMETRY PARAMETERS  = .02000 .00000 .00000
                      .00000 .00000 .00000
HALFWIDTH PARAMETERS U = .874376 -.000104 .069463
                      V = -.005000 .000000 .000000
                      W = .020000 .000000 .000000
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000
EXTINCTION PARAMETER   = .000000 .000000 .000000

```

MOLAR PERCENTAGE OF PHASES:

```

PHASE 1:  -5.17 .67
PHASE 2:  105.17 3.76

```

WEIGHT PERCENTAGE OF PHASES:

```

-8.23 1.07
108.23 4.02

```

```

+-----+
| Hist | Rp | Rwp | Rexp |Durbin Unwght| Durbin Wght | N-P |
+-----+
| 1 | 12.72 | 17.62 | 10.78 | .506 | .515 | 5285 |
+-----+

```

	SUMYDIF		SUMYOBS		SUMYCALC		SUMWYOBSSQ		GOF		CONDITION	
+	-----+											
	.5783E+05		.4546E+06		.4330E+06		.4546E+06		.2671E+01		.1322E+12	
+	-----+											

+++++

+++++

CYCLE NUMBER= 7

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
ZR	.27580	.00000	.00000	.04110	.00000	.00000	.20820	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.07030	.00000	.00000	.33590	.00000	.00000	.34060	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.44230	.00000	.00000	.75490	.00000	.00000	.47890	.00000	.00000	
.5000	.0000	.0000	1.0000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

-----+

| Phase: 1 |

-----+

PHASE SCALE FACTOR = -.278635E-05 .229609E-05 .532745E-06

OVERALL TEMP. FACTOR = .000000 .000000 .000000

CELL PARAMETERS = 5.145000 .000000 .000000

5.207000 .000000 .000000

5.311000 .000000 .000000

90.000010 .000000 .000000

99.200000 .000000 .000000

90.000010 .000000 .000000

RECIPROCAL CELL = .197 .192 .191 90.000 80.800 90.000

CELL VOLUME = 140.451500 .000000

SCALE \* VOLUME = -.000391 .000075

MOLECULAR WEIGHT = 492.880

DENSITY = 5.825

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = -129.444

-----+

| Histogram: 1 |

-----+

SCALE FACTOR = 1.0000 .00000 .00000

ZEROPOINT = .00000 .00000 .00000

SAMPLE DISPLACEMENT	=	-.52575	-.00002	.00628	
BACKGROUND PARAMETER B 0	=	81.2862	.170969E-03	.180068	
PREFERRED ORIENTATION	=	1.00000	.00000	.00000	
ABSORPTION R	=	.00000	.00000	.00000	
ASYMMETRY PARAMETERS	=	.02000	.00000	.00000	
		.00000	.00000	.00000	
HALFWIDTH PARAMETERS U	=	-.840141	-.000182	.005765	
V	=	.869971	.000048	.006377	
W	=	.020000	.000000	.000000	
ANISOTROPIC GAUSSIAN BROADENING	=	.000000	.000000	.000000	
PEAK SHAPE PARAMETER Gam0	=	.200000	.000000	.000000	
PEAK SHAPE PARAMETER Gam1	=	.000000	.000000	.000000	
PEAK SHAPE PARAMETER Gam2	=	.000000	.000000	.000000	
EXTINCTION PARAMETER	=	.000000	.000000	.000000	

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33	SB33	
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23	SB23	
SB23										
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

```

+-----+
|                               |
|                               |
+-----+

```

PHASE SCALE FACTOR	=	.179258E-03	-.808976E-09	.357959E-05
OVERALL TEMP. FACTOR	=	.000000	.000000	.000000
CELL PARAMETERS	=	4.683700	.000000	.000000
		3.422600	.000000	.000000
		5.128799	.000000	.000000
		90.000010	.000000	.000000
		99.540010	.000000	.000000
		90.000010	.000000	.000000
RECIPROCAL CELL	=	.217	.292	.198
CELL VOLUME	=	81.079820	.000000	
SCALE * VOLUME	=	.014534	.000290	
MOLECULAR WEIGHT	=	318.200		
DENSITY	=	6.514		

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM<sup>2</sup> ( in cm<sup>-2</sup>)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = 3103.63

```

+-----+
|                               |
|                               |
+-----+

```

SCALE FACTOR	=	1.0000	.00000	.00000
ZEROPOINT	=	.00000	.00000	.00000

SAMPLE DISPLACEMENT	=	-.52575	-.00002	.00628	
BACKGROUND PARAMETER B 0	=	81.2862	.170969E-03	.180068	
PREFERRED ORIENTATION	=	1.00000	.00000	.00000	
ABSORPTION R	=	.00000	.00000	.00000	
ASYMMETRY PARAMETERS	=	.02000	.00000	.00000	
		.00000	.00000	.00000	
HALFWIDTH PARAMETERS U	=	.874464	.000088	.057308	
V	=	-.005000	.000000	.000000	
W	=	.020000	.000000	.000000	
ANISOTROPIC GAUSSIAN BROADENING	=	.000000	.000000	.000000	
PEAK SHAPE PARAMETER Gam0	=	.200000	.000000	.000000	
PEAK SHAPE PARAMETER Gam1	=	.000000	.000000	.000000	
PEAK SHAPE PARAMETER Gam2	=	.000000	.000000	.000000	
EXTINCTION PARAMETER	=	.000000	.000000	.000000	

MOLAR PERCENTAGE OF PHASES:			WEIGHT PERCENTAGE OF PHASES:	
PHASE 1:	-2.77	.53	-4.35	.84
PHASE 2:	102.77	2.99	104.35	3.13

Hist	Rp	Rwp	Rexp	Durbin Unwght	Durbin Wght	N-P
1	11.58	14.54	10.78	.705	.756	5285

  

SUMYDIF	SUMYOBS	SUMYCALC	SUMWYOBSQ	GOF	CONDITION
.5264E+05	.4546E+06	.4439E+06	.4546E+06	.1818E+01	.1322E+12

+++++

CYCLE NUMBER= 8

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
ZR	.27580	.00000	.00000	.04110	.00000	.00000	.20820	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.07030	.00000	.00000	.33590	.00000	.00000	.34060	.00000	.00000	
1.0000	.0000	.0000	1.0000	.0000	.0000					
O	.44230	.00000	.00000	.75490	.00000	.00000	.47890	.00000	.00000	
.5000	.0000	.0000	1.0000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

Phase: 1
----------

PHASE SCALE FACTOR = -.255786E-05 .228488E-06 .531551E-06

OVERALL TEMP. FACTOR = .000000 .000000 .000000  
CELL PARAMETERS = 5.145000 .000000 .000000  
5.207000 .000000 .000000  
5.311000 .000000 .000000  
90.000010 .000000 .000000  
99.200000 .000000 .000000  
90.000010 .000000 .000000  
RECIPROCAL CELL = .197 .192 .191 90.000 80.800 90.000  
CELL VOLUME = 140.451500 .000000  
SCALE \* VOLUME = -.000359 .000075  
MOLECULAR WEIGHT = 492.880  
DENSITY = 5.825

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM<sup>2</sup> ( in cm<sup>-2</sup>)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = -118.829

+-----+  
| Histogram: 1 |  
+-----+

SCALE FACTOR = 1.0000 .00000 .00000  
ZEROPOINT = .00000 .00000 .00000  
SAMPLE DISPLACEMENT = -.52538 .00037 .00721  
BACKGROUND PARAMETER B 0 = 81.2863 .927984E-04 .179648  
PREFERRED ORIENTATION = 1.00000 .00000 .00000  
ABSORPTION R = .00000 .00000 .00000  
ASYMMETRY PARAMETERS = .02000 .00000 .00000  
.00000 .00000 .00000  
HALFWIDTH PARAMETERS U = -.840519 -.000378 .010498  
V = .870111 .000140 .011612  
W = .020000 .000000 .000000  
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000  
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000  
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000  
PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000  
EXTINCTION PARAMETER = .000000 .000000 .000000

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	

+-----+  
| Phase: 2 |  
+-----+

PHASE SCALE FACTOR = .179260E-03 .226349E-08 .357134E-05  
 OVERALL TEMP. FACTOR = .000000 .000000 .000000  
 CELL PARAMETERS = 4.683700 .000000 .000000  
                   3.422600 .000000 .000000  
                   5.128799 .000000 .000000  
                   90.000010 .000000 .000000  
                   99.540010 .000000 .000000  
                   90.000010 .000000 .000000  
 RECIPROCAL CELL = .217 .292 .198 90.000 80.460 90.000  
 CELL VOLUME = 81.079820 .000000  
 SCALE \* VOLUME = .014534 .000290  
 MOLECULAR WEIGHT = 318.200  
 DENSITY = 6.514

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)  
 MASS = MASS OF PHASE IN BEAM (in g)  
 ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = 3103.67

```

+-----+
| Histogram: 1 |
+-----+
SCALE FACTOR = 1.0000 .00000 .00000
ZEROPOINT = .00000 .00000 .00000

SAMPLE DISPLACEMENT = -.52538 .00037 .00721

BACKGROUND PARAMETER B 0 = 81.2863 .927984E-04 .179648
PREFERRED ORIENTATION = 1.00000 .00000 .00000
ABSORPTION R = .00000 .00000 .00000
ASYMMETRY PARAMETERS = .02000 .00000 .00000
                     .00000 .00000 .00000
HALFWIDTH PARAMETERS U = .874491 .000027 .057179
                       V = -.005000 .000000 .000000
                       W = .020000 .000000 .000000
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000
EXTINCTION PARAMETER = .000000 .000000 .000000
  
```

MOLAR PERCENTAGE OF PHASES:

PHASE 1: -2.53 .53  
 PHASE 2: 102.53 2.98

WEIGHT PERCENTAGE OF PHASES:

-3.98 .83  
 103.98 3.11

```

+-----+
| Hist | Rp | Rwp | Rexp | Durbin Unwght | Durbin Wght | N-P |
+-----+
| 1 | 11.54 | 14.50 | 10.78 | .710 | .761 | 5285 |
+-----+
| SUMYDIF | SUMYOBS | SUMYCALC | SUMWYOBSQ | GOF | CONDITION |
+-----+
| .5246E+05 | .4546E+06 | .4449E+06 | .4546E+06 | .1810E+01 | .1322E+12 |
+-----+
  
```

+-----+  
 +-----+

CYCLE NUMBER= 9

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						



ZR	.27580	.00000	.00000	.04110	.00000	.00000	.20820	.00000	.00000
1.0000	.0000	.0000	1.0000	.0000	.0000				
O	.07030	.00000	.00000	.33590	.00000	.00000	.34060	.00000	.00000
1.0000	.0000	.0000	1.0000	.0000	.0000				
O	.44230	.00000	.00000	.75490	.00000	.00000	.47890	.00000	.00000
.5000	.0000	.0000	1.0000	.0000	.0000				
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33	
SB33									
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23	
SB23									
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000									

```

+-----+
|                               |
|                               |
+-----+

```

```

PHASE SCALE FACTOR   = -.253591E-05 .219524E-07 .531560E-06
OVERALL TEMP. FACTOR = .000000 .000000 .000000
CELL PARAMETERS      =  5.145000 .000000 .000000
                      =  5.207000 .000000 .000000
                      =  5.311000 .000000 .000000
                      = 90.000010 .000000 .000000
                      = 99.200000 .000000 .000000
                      = 90.000010 .000000 .000000
RECIPROCAL CELL      =  .197 .192 .191 90.000 80.800 90.000
CELL VOLUME          = 140.451500 .000000
SCALE * VOLUME       =  -.000356 .000075
MOLECULAR WEIGHT     =  492.880
DENSITY              =  5.825

```

ABSOLUTE PHASE VALUES:

```

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
MASS = MASS OF PHASE IN BEAM (in g)
ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

```

Then:

INC\*MASS\*ls/R = -117.809

```

+-----+
|                               |
|                               |
+-----+

```

```

SCALE FACTOR          = 1.0000 .00000 .00000
ZEROPOINT             = .00000 .00000 .00000

SAMPLE DISPLACEMENT   = -.52529 .00010 .00730

BACKGROUND PARAMETER B 0 = 81.2864 .667647E-04 .179645
PREFERRED ORIENTATION  = 1.00000 .00000 .00000
ABSORPTION R          = .00000 .00000 .00000
ASYMMETRY PARAMETERS  = .02000 .00000 .00000
                      = .00000 .00000 .00000
HALFWIDTH PARAMETERS U = -.840036 .000483 .011310
                      V = .869288 -.000822 .012513
                      W = .020000 .000000 .000000
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000
EXTINCTION PARAMETER  = .000000 .000000 .000000

```

PHASE 2: CuO  
NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
1.0000	.0000	.0000	.5000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

+-----+  
| Phase: 2 |  
+-----+

PHASE SCALE FACTOR = .179261E-03 .797811E-09 .357129E-05  
OVERALL TEMP. FACTOR = .000000 .000000 .000000  
CELL PARAMETERS = 4.683700 .000000 .000000  
3.422600 .000000 .000000  
5.128799 .000000 .000000  
90.000010 .000000 .000000  
99.540010 .000000 .000000  
90.000010 .000000 .000000  
RECIPROCAL CELL = .217 .292 .198 90.000 80.460 90.000  
CELL VOLUME = 81.079820 .000000  
SCALE \* VOLUME = .014534 .000290  
MOLECULAR WEIGHT = 318.200  
DENSITY = 6.514

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM<sup>2</sup> ( in cm<sup>-2</sup>)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = 3103.68

+-----+  
| Histogram: 1 |  
+-----+

SCALE FACTOR = 1.0000 .00000 .00000  
ZEROPOINT = .00000 .00000 .00000  
SAMPLE DISPLACEMENT = -.52529 .00010 .00730  
BACKGROUND PARAMETER B 0 = 81.2864 .667647E-04 .179645  
PREFERRED ORIENTATION = 1.00000 .00000 .00000  
ABSORPTION R = .00000 .00000 .00000  
ASYMMETRY PARAMETERS = .02000 .00000 .00000  
.00000 .00000 .00000  
HALFWIDTH PARAMETERS U = .874474 -.000016 .057177  
V = -.005000 .000000 .000000  
W = .020000 .000000 .000000  
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000  
PEAK SHAPE PARAMETER Gam0 = .200000 .000000 .000000  
PEAK SHAPE PARAMETER Gam1 = .000000 .000000 .000000  
PEAK SHAPE PARAMETER Gam2 = .000000 .000000 .000000

MOLAR PERCENTAGE OF PHASES:			WEIGHT PERCENTAGE OF PHASES:	
PHASE 1:	-2.51	.53	-3.95	.83
PHASE 2:	102.51	2.97	103.95	3.11

Hist	Rp	Rwp	Rexp	Durbin Unwght	Durbin Wght	N-P
1	11.54	14.50	10.78	.711	.761	5285
SUMYDIF	SUMYOBS	SUMYCALC	SUMWYOBSSQ	GOF	CONDITION	
.5245E+05	.4546E+06	.4451E+06	.4546E+06	.1810E+01	.1322E+12	

	1	2	3	4	5	6	7
1	100	1	-3	1	0	1	0
2	1	100	-24	0	1	-21	-12
3	-3	-24	100	0	1	-7	-7
4	1	0	0	100	-99	0	0
5	0	1	1	-99	100	0	0
6	1	-21	-7	0	0	100	45
7	0	-12	-7	0	0	45	100

		1	21.7	2	19.4	3	14.1	4	9.6	5	6.7	6	7.7	7	7.3
8	4.5	9	1.0	10	-.7										
		11	1.2	12	.9	13	-4.6	14	-10.9	15	-7.9	16	-7.4	17	-7.9
18	-12.1	19	-13.5	20	-12.3										
		21	-8.3	22	-.1	23	-10.4	24	-11.4	25	-10.1	26	-8.0	27	-8.1
28	-7.6	29	-8.5	30	-8.9										
		31	-5.9	32	-6.4	33	-4.9	34	-3.6	35	-3.3	36	-.5	37	1.5
38	1.0	39	-4.2	40	-1.4										
		41	-3.0	42	2.6	43	2.8	44	-1.7	45	1.7	46	-.8	47	.6
48	.2	49	1.8	50	1.8										
		51	3.6	52	-.5	53	2.4	54	5.4	55	14.4	56	3.4	57	-.1
58	.9	59	4.9	60	28.0										
		61	32.0	62	10.4	63	6.1	64	9.3	65	2.1	66	3.4	67	-4.9
68	-6.4	69	-2.7	70	-5.2										
		71	-4.6	72	-.9	73	-.2	74	5.2	75	2.9	76	-18.8	77	-6.8
78	5.8	79	-10.5	80	-11.0										
		81	-15.2	82	-14.3	83	-7.7	84	-3.9	85	6.5	86	-12.3	87	1.7
88	-6.7	89	-9.9	90	-7.8										
		91	-5.3	92	-4.5	93	-4.2	94	-8.4	95	-9.5	96	-10.1	97	-9.0
98	-11.3	99	-8.2	100	-7.8										
		101	-10.0	102	-9.8	103	-11.0	104	-8.1	105	-12.2	106	-12.7	107	-9.9
-7.6	109	-8.7	110	-12.3											
		111	-12.0	112	-15.0	113	-9.0	114	-11.8	115	-6.0	116	21.2	117	8.0
.2	119	16.2	120	33.1											
		121	18.3	122	9.3	123	-2.4	124	-8.4	125	-8.8	126	-9.2	127	-7.1
-6.4	129	-4.8	130	-3.9											
		131	-2.8	132	-3.6	133	-3.7	134	-3.3	135	-.2	136	1.9	137	-2.5
-8.2	139	-1.5	140	-2.5											
		141	-2.3	142	.5	143	11.4	144	3.2	145	1.5	146	11.6	147	8.3
7.9	149	24.9	150	16.9											
		151	2.9	152	3.8	153	33.0	154	15.3	155	.7	156	3.8	157	7.7
.2	159	-3.0	160	-3.0											
		161	-1.0	162	.1	163	-.1	164	1.0	165	12.3	166	23.2	167	27.9
20.4	169	4.6	170	-1.5											
		171	5.6	172	30.0	173	16.0	174	2.3	175	2.3	176	-2.5	177	-.2
.9	179	-4.2	180	-3.2											
		181	-.7	182	.8	183	.7	184	2.2	185	10.8	186	6.9	187	3.7
-.3	189	5.5	190	.2											
		191	6.4	192	12.9	193	22.3	194	10.0	195	5.0	196	-.1	197	5.8

		201	1.7	202	-.9	203	-1.3	204	3.5	205	4.0	206	.3	207	-1.3	208
7.6	209	7.2	210	3.1												
		211	7.1	212	15.4	213	13.6	214	14.4	215	18.5	216	15.6	217	8.5	218
9.5	219	5.3	220	3.0												
		221	9.6	222	.1	223	6.1	224	3.2	225	.7	226	.6	227	8.9	228
-1.9	229	3.7	230	2.9												
		231	3.4	232	7.0	233	4.2	234	.3	235	7.3	236	8.7	237	8.0	238
3.7	239	.1	240	2.1												
		241	1.5	242	13.8	243	2.4	244	-1.9	245	4.6	246	.9	247	5.5	248
6.3	249	10.3	250	9.9												
		251	7.7	252	8.4	253	14.8	254	7.3	255	9.5	256	6.1	257	5.6	258
5.3	259	7.0	260	10.7												
		261	7.0	262	12.2	263	6.4	264	13.4	265	49.4					
NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD					
4.1	1	1	0	1	0	.362	.200	17.015	-207.	-204.	3.2					
2.1	2	2	0	1	0	.363	.200	17.057	-103.	-101.	1.4					
.1	3	1	1	0	0	.366	.200	17.447	-7.	-6.	.9					
.1	4	2	1	0	0	.366	.200	17.491	-4.	-3.	.5					
.3	5	1	0	1	-1	.409	.200	24.069	-15.	-16.	-.7					
.3	6	1	0	1	1	.409	.200	24.069	-15.	-16.	-.7					
.1	7	2	0	1	-1	.409	.200	24.129	-8.	-8.	-.3					
.1	8	2	0	1	1	.409	.200	24.129	-8.	-8.	-.3					
.2	9	1	1	1	0	.411	.200	24.464	-14.	-14.	.1					
.1	10	2	1	1	0	.412	.200	24.525	-7.	-7.	.1					
.0	11	1	1	1	-1	.431	.200	28.201	0.	0.	.0					
.0	12	2	1	1	-1	.431	.200	28.271	0.	0.	.0					
.1	13	1	1	1	1	.446	.200	31.483	-5.	-5.	-.4					
.0	14	2	1	1	1	.446	.200	31.562	-2.	-2.	-.2					
.4	15	1	0	0	2	.456	.200	34.178	-26.	-26.	.2					
.2	16	2	0	0	2	.456	.200	34.265	-13.	-13.	.1					
.3	17	1	0	2	0	.457	.200	34.420	-16.	-16.	.0					
.1	18	2	0	2	0	.457	.200	34.507	-8.	-8.	-.1					
.3	19	1	2	0	0	.460	.200	35.316	-20.	-19.	.5					
.1	20	2	2	0	0	.461	.200	35.406	-10.	-9.	.5					
.1	21	1	1	0	-2	.462	.200	35.924	-4.	-4.	-.1					
.0	22	2	1	0	-2	.463	.200	36.016	-2.	-2.	-.1					
.3	23	1	0	1	-2	.470	.200	38.415	-20.	-20.	-.3					
.3	24	1	0	1	2	.470	.200	38.415	-20.	-20.	-.3					
.1	25	2	0	1	-2	.471	.200	38.514	-10.	-10.	-.2					
.1	26	2	0	1	2	.471	.200	38.514	-10.	-10.	-.2					

.0	27	1	0	2	-1	.471	.200	38.579	-4.	-4.	-.1	
.0	28	1	0	2	1	.471	.200	38.579	-4.	-4.	-.1	
.0	29	2	0	2	-1	.471	.200	38.678	-2.	-2.	.0	
.0	30	2	0	2	1	.471	.200	38.678	-2.	-2.	.0	
.0	31	1	1	2	0	.471	.200	38.839	0.	0.	.0	
.0	32	2	1	2	0	.472	.200	38.938	0.	0.	.0	
.9	33	1	2	1	0	.473	.200	39.448	-56.	-54.	1.8	
.4	34	2	2	1	0	.473	.200	39.549	-28.	-26.	1.8	
.4	35	1	1	1	-2	.475	.200	40.002	-26.	-23.	2.9	
.2	36	2	1	1	-2	.475	.200	40.105	-13.	-12.	1.3	
.0	37	1	2	1	-1	.477	.200	40.753	0.	0.	.0	
.0	38	2	2	1	-1	.477	.200	40.858	0.	0.	.0	
.1	39	1	1	0	2	.478	.200	41.168	-6.	-6.	.4	
.0	40	2	1	0	2	.478	.200	41.274	-3.	-3.	.2	
.1	41	1	1	2	-1	.478	.200	41.411	-7.	-6.	.5	
.0	42	2	1	2	-1	.479	.200	41.517	-3.	-3.	.3	
.0	43	1	1	2	1	.484	.200	43.823	0.	0.	.0	
.0	44	2	1	2	1	.484	.200	43.936	0.	0.	.0	
.1	45	1	1	1	2	.486	.200	44.845	-5.	-4.	.6	
.0	46	2	1	1	2	.486	.200	44.961	-2.	-2.	.3	
.1	47	1	2	1	1	.487	.200	45.531	-5.	-4.	.8	
.1	48	1	2	0	-2	.487	.200	45.551	-8.	-7.	1.2	
.0	49	2	2	1	1	.487	.200	45.649	-3.	-2.	.4	
.1	50	2	2	0	-2	.487	.200	45.669	-4.	-3.	.6	
	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
.2	51	1	2	1	-2	.492	.200	48.966	-16.	-18.	-2.0	
.1	52	2	2	1	-2	.492	.200	49.095	-8.	-9.	-1.1	
.2	53	1	0	2	-2	.492	.200	49.291	-11.	-13.	-1.3	
.2	54	1	0	2	2	.492	.200	49.291	-11.	-13.	-1.3	
.1	55	2	0	2	-2	.492	.200	49.420	-6.	-6.	-.5	
.1	56	2	0	2	2	.492	.200	49.420	-6.	-6.	-.5	
.5	57	1	2	2	0	.493	.200	50.142	-28.	-34.	-6.6	
.3	58	2	2	2	0	.493	.200	50.274	-14.	-18.	-4.2	

.3	59	1	1	2	-2	.493	.200	50.601	-16.	-21.	-4.7
.1	60	2	1	2	-2	.494	.200	50.735	-8.	-10.	-2.0
.1	61	1	2	2	-1	.494	.200	51.228	-7.	-8.	-.4
.1	62	2	2	2	-1	.494	.200	51.363	-4.	-4.	.0
.1	63	1	0	3	0	.495	.200	52.694	-9.	-8.	.8
.1	64	2	0	3	0	.495	.200	52.834	-4.	-4.	.4
.2	65	1	2	0	2	.495	.200	54.108	-14.	-13.	.6
.0	66	1	3	0	0	.495	.200	54.131	-2.	-2.	.1
.1	67	2	2	0	2	.495	.200	54.252	-7.	-7.	.2
.0	68	2	3	0	0	.495	.200	54.275	-1.	-1.	.0
.0	69	1	1	2	2	.495	.200	54.711	-1.	-1.	.0
.0	70	2	1	2	2	.495	.200	54.857	0.	0.	.0
.1	71	1	2	2	1	.495	.200	55.305	-5.	-5.	.1
.0	72	1	0	1	-3	.495	.200	55.414	0.	0.	.0
.0	73	1	0	1	3	.495	.200	55.414	0.	0.	.0
.0	74	2	2	2	1	.495	.200	55.452	-3.	-3.	.0
.0	75	2	0	1	-3	.495	.200	55.562	0.	0.	.0
.0	76	2	0	1	3	.495	.200	55.562	0.	0.	.0
.0	77	1	1	1	-3	.495	.200	55.640	-1.	-1.	.0
.1	78	1	0	3	-1	.495	.200	55.744	-5.	-5.	.0
.1	79	1	0	3	1	.495	.200	55.744	-5.	-5.	.0
.0	80	2	1	1	-3	.495	.200	55.789	0.	0.	.0
.0	81	2	0	3	-1	.495	.200	55.893	-2.	-2.	.0
.0	82	2	0	3	1	.495	.200	55.893	-2.	-2.	.0
.0	83	1	1	3	0	.495	.200	55.940	0.	0.	.0
.0	84	2	1	3	0	.495	.200	56.089	0.	0.	.0
.2	85	1	2	1	2	.495	.200	57.147	-15.	-15.	.3
.1	86	1	3	1	0	.495	.200	57.169	-3.	-3.	.1
.0	87	1	3	1	-1	.495	.200	57.197	0.	0.	.0
.1	88	2	2	1	2	.494	.200	57.300	-7.	-7.	.2
.0	89	2	3	1	0	.494	.200	57.322	-2.	-2.	.0
.0	90	2	3	1	-1	.494	.200	57.351	0.	0.	.0
.0	91	1	1	3	-1	.494	.200	57.917	-1.	-1.	.0

.0	92	2	1	3	-1	.494	.200	58.074	-1.	-1.	.0	
.1	93	1	2	2	-2	.494	.200	58.319	-4.	-5.	-.4	
.0	94	2	2	2	-2	.494	.200	58.476	-2.	-2.	-.1	
.0	95	1	1	3	1	.492	.200	59.825	0.	0.	.0	
.0	96	2	1	3	1	.492	.200	59.988	0.	0.	.0	
.2	97	1	3	0	-2	.492	.200	60.083	-9.	-11.	-1.7	
.1	98	2	3	0	-2	.492	.200	60.246	-4.	-6.	-1.1	
.0	99	1	1	1	3	.490	.200	61.387	0.	0.	.0	
.0	100	2	1	1	3	.490	.200	61.555	0.	0.	.0	
	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
.0	101	1	2	1	-3	.489	.200	62.022	0.	0.	.0	
.0	102	2	2	1	-3	.489	.200	62.192	0.	0.	.0	
.0	103	1	3	1	1	.488	.200	62.856	0.	0.	.0	
.1	104	1	3	1	-2	.488	.200	62.937	-7.	-8.	-.5	
.0	105	2	3	1	1	.487	.200	63.028	0.	0.	.0	
.1	106	2	3	1	-2	.487	.200	63.110	-4.	-4.	-.2	
.0	107	1	0	2	-3	.485	.200	64.130	-1.	-1.	.0	
.0	108	1	0	2	3	.485	.200	64.130	-1.	-1.	.0	
.0	109	2	0	2	-3	.485	.200	64.306	0.	0.	.0	
.0	110	2	0	2	3	.485	.200	64.306	0.	0.	.0	
.0	111	1	0	3	-2	.485	.200	64.319	-3.	-3.	.0	
.0	112	1	0	3	2	.485	.200	64.319	-3.	-3.	.0	
.0	113	1	1	2	-3	.485	.200	64.337	-2.	-2.	.0	
.0	114	2	0	3	-2	.484	.200	64.496	-1.	-1.	.0	
.0	115	2	0	3	2	.484	.200	64.496	-1.	-1.	.0	
.0	116	2	1	2	-3	.484	.200	64.514	-1.	-1.	.0	
.1	117	1	2	3	0	.483	.200	65.036	-4.	-4.	.0	
.0	118	2	2	3	0	.482	.200	65.216	-2.	-2.	.0	
.0	119	1	1	3	-2	.482	.200	65.426	-1.	-1.	.0	
.0	120	2	1	3	-2	.481	.200	65.607	-1.	-1.	-.1	
.1	121	1	2	2	2	.481	.200	65.721	-6.	-7.	-.8	
.0	122	1	3	2	0	.481	.200	65.741	-2.	-3.	-.3	
.0	123	1	3	2	-1	.481	.200	65.768	-1.	-1.	-.1	

.0	124	2	2	2	2	.480	.200	65.903	-3.	-4.	-.6
.0	125	2	3	2	0	.480	.200	65.924	-1.	-1.	-.2
.0	126	2	3	2	-1	.480	.200	65.950	0.	0.	-.1
.1	127	1	2	3	-1	.480	.200	65.960	-5.	-6.	-.9
.0	128	2	2	3	-1	.480	.200	66.143	-2.	-3.	-.5
.0	129	1	1	3	2	.470	.200	68.970	-1.	-1.	.0
.0	130	2	1	3	2	.469	.200	69.164	0.	0.	.0
.0	131	1	2	3	1	.468	.200	69.490	-3.	-3.	.1
.0	132	1	1	2	3	.467	.200	69.661	-1.	-1.	.0
.0	133	2	2	3	1	.467	.200	69.686	-2.	-2.	.0
.0	134	2	1	2	3	.467	.200	69.857	-1.	-1.	.0
.0	135	1	2	2	-3	.465	.200	70.256	-1.	-1.	.0
.0	136	2	2	2	-3	.464	.200	70.455	0.	0.	.0
.0	137	1	3	0	2	.462	.200	70.869	0.	0.	.0
.0	138	1	3	2	1	.461	.200	71.039	0.	0.	.0
.0	139	2	3	0	2	.461	.200	71.070	0.	0.	.0
.0	140	1	3	2	-2	.461	.200	71.115	-3.	-3.	.0
.0	141	2	3	2	1	.460	.200	71.240	0.	0.	.0
.0	142	2	3	2	-2	.460	.200	71.317	-1.	-1.	.0
.1	143	1	1	0	-4	.460	.200	71.326	-5.	-5.	.0
.0	144	2	1	0	-4	.459	.200	71.528	-3.	-3.	.0
.0	145	1	0	0	4	.457	.200	71.990	-1.	-1.	.0
.0	146	1	2	3	-2	.456	.200	72.161	-1.	-1.	.0
.0	147	2	0	0	4	.456	.200	72.195	-1.	-1.	.0
.0	148	2	2	3	-2	.455	.200	72.366	0.	0.	.0
.0	149	1	0	4	0	.454	.200	72.561	-1.	-1.	-.1
.0	150	1	2	1	3	.453	.200	72.656	0.	0.	.0
NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
.0	151	2	0	4	0	.453	.200	72.769	-1.	-1.	-.1
.0	152	2	2	1	3	.452	.200	72.863	0.	0.	.0
.0	153	1	3	1	2	.448	.200	73.504	0.	0.	.0
.0	154	1	3	1	-3	.448	.200	73.630	-1.	-1.	.0
.0	155	2	3	1	2	.447	.200	73.714	0.	0.	.0



.0	156	2	3	1	-3	.446	.200	73.841	-1.	-1.	.0
.1	157	1	1	1	-4	.446	.200	73.954	-6.	-6.	-.3
.0	158	2	1	1	-4	.444	.200	74.166	-3.	-3.	-.1
.0	159	1	0	1	-4	.442	.200	74.608	-1.	-1.	-.1
.0	160	1	0	1	4	.442	.200	74.608	-1.	-1.	-.1
.0	161	1	4	0	0	.441	.200	74.699	-2.	-2.	-.2
.0	162	2	0	1	-4	.440	.200	74.823	0.	-1.	-.1
.0	163	2	0	1	4	.440	.200	74.823	0.	-1.	-.1
.0	164	2	4	0	0	.440	.200	74.914	-1.	-1.	-.2
.1	165	1	0	4	-1	.438	.200	75.137	-3.	-4.	-.6
.1	166	1	0	4	1	.438	.200	75.137	-3.	-4.	-.6
.0	167	1	1	4	0	.437	.200	75.305	-1.	-1.	-.1
.0	168	2	0	4	-1	.437	.200	75.354	-1.	-2.	-.3
.0	169	2	0	4	1	.437	.200	75.354	-1.	-2.	-.3
.0	170	2	1	4	0	.436	.200	75.523	0.	0.	.0
.0	171	1	2	0	-4	.431	.200	76.163	0.	0.	.0
.0	172	2	2	0	-4	.429	.200	76.384	0.	0.	.0
.0	173	1	4	1	-1	.429	.200	76.470	-1.	-1.	.0
.0	174	2	4	1	-1	.427	.200	76.693	0.	0.	.0
.0	175	1	1	4	-1	.425	.200	77.012	0.	0.	.0
.0	176	2	1	4	-1	.423	.200	77.236	0.	0.	.0
.1	177	1	4	1	0	.422	.200	77.284	-4.	-4.	-.1
.0	178	1	0	3	-3	.421	.200	77.439	-1.	-1.	.0
.0	179	1	0	3	3	.421	.200	77.439	-1.	-1.	.0
.0	180	2	4	1	0	.421	.200	77.510	-2.	-2.	.0
.0	181	1	1	3	-3	.420	.200	77.629	-2.	-2.	.0
.0	182	2	0	3	-3	.419	.200	77.665	0.	0.	.0
.0	183	2	0	3	3	.419	.200	77.665	0.	0.	.0
.0	184	2	1	3	-3	.418	.200	77.856	-1.	-1.	.0
.0	185	1	1	0	4	.416	.200	78.102	-1.	-1.	.0
.0	186	1	4	0	-2	.415	.200	78.159	-1.	-1.	.0
.0	187	2	1	0	4	.414	.200	78.331	-1.	0.	.0
.0	188	2	4	0	-2	.413	.200	78.388	0.	0.	.0



.0	221	1	4	1	1	.362	.200	83.112	0.	0.	.0	
.0	222	1	2	3	-3	.361	.200	83.167	0.	0.	-.1	
.0	223	1	2	4	0	.358	.200	83.359	-1.	-1.	-.1	
.0	224	2	4	1	1	.358	.200	83.362	0.	0.	.0	
.0	225	2	2	3	-3	.358	.200	83.418	0.	0.	.0	
.0	226	2	2	4	0	.355	.200	83.610	0.	-1.	-.1	
.0	227	1	1	4	-2	.353	.200	83.715	0.	0.	.0	
.0	228	1	3	3	1	.351	.200	83.911	0.	0.	.0	
.0	229	2	1	4	-2	.350	.200	83.968	0.	0.	.0	
.0	230	1	3	3	-2	.350	.200	83.984	-3.	-3.	-.2	
.0	231	1	4	2	-1	.348	.200	84.109	0.	0.	.0	
.0	232	2	3	3	1	.347	.200	84.164	0.	0.	.0	
.0	233	1	2	4	-1	.346	.200	84.204	-2.	-2.	-.1	
.0	234	2	3	3	-2	.346	.200	84.238	-1.	-1.	-.1	
.0	235	2	4	2	-1	.344	.200	84.364	0.	0.	.0	
.0	236	2	2	4	-1	.342	.200	84.459	-1.	-1.	-.1	
.0	237	1	4	2	0	.336	.200	84.905	-2.	-2.	-.2	
.0	238	2	4	2	0	.331	.200	85.163	-1.	-1.	.0	
.0	239	1	3	0	-4	.313	.200	86.208	-2.	-2.	.0	
.0	240	1	2	2	-4	.311	.200	86.326	0.	0.	.0	
.0	241	2	3	0	-4	.308	.200	86.472	-1.	-1.	.0	
.0	242	2	2	2	-4	.306	.200	86.590	0.	0.	.0	
.0	243	1	1	4	2	.298	.200	86.992	0.	0.	.0	
.0	244	2	1	4	2	.293	.200	87.260	0.	0.	.0	
.1	245	1	2	4	1	.288	.200	87.480	-3.	-3.	-.2	
.0	246	2	2	4	1	.282	.200	87.750	-2.	-2.	.0	
.1	247	1	1	2	4	.271	.200	88.218	-3.	-3.	-.1	
.0	248	1	4	2	-2	.270	.200	88.274	-1.	-1.	.0	
.0	249	2	1	2	4	.265	.200	88.492	-1.	-2.	-.1	
.0	250	2	4	2	-2	.263	.200	88.548	0.	0.	.0	
	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
.0	251	1	3	1	3	.263	.200	88.549	0.	0.	.0	
.1	252	1	3	1	-4	.259	.200	88.718	-4.	-4.	-.2	

.0	253	2	3	1	3	.256	.200	88.824	0.	0.	.0
.0	254	2	3	1	-4	.252	.200	88.994	-2.	-2.	-.1
.0	255	1	2	0	4	.242	.200	89.362	-1.	-2.	-.1
.0	256	2	2	0	4	.234	.200	89.641	-1.	-1.	-.1
.0	257	1	4	1	-3	.227	.200	89.854	0.	0.	.0
.0	258	1	2	4	-2	.223	.200	90.002	-1.	-1.	-.1
.0	259	2	4	1	-3	.218	.200	90.135	0.	0.	.0
.0	260	2	2	4	-2	.213	.200	90.285	-1.	-1.	.0
.0	261	1	4	2	1	.201	.200	90.652	-1.	-1.	.0
.0	262	2	4	2	1	.190	.200	90.937	-1.	-1.	.0
.0	263	1	4	0	2	.174	.200	91.308	-2.	-2.	.0
.0	264	2	4	0	2	.161	.200	91.597	-1.	-1.	.0
.1	265	1	2	1	4	.148	.200	91.870	-2.	-2.	-.3
.0	266	2	2	1	4	.131	.200	92.161	-1.	-1.	-.1
.1	267	1	2	3	3	.062	.200	92.984	-2.	-2.	.1
.1	268	2	2	3	3	.010	.200	93.281	-1.	-1.	-.1
.0	269	1	3	3	2	.010	.200	93.796	0.	0.	.0
.4	270	1	4	1	2	.010	.200	93.819	-4.	-4.	-.4
.1	271	1	3	3	-3	.010	.200	93.917	-1.	-2.	-.2
.0	272	2	3	3	2	.010	.200	94.098	0.	0.	.0
.2	273	2	4	1	2	.010	.200	94.120	-2.	-3.	-.5
.1	274	2	3	3	-3	.010	.200	94.219	-1.	-1.	.0
.2	275	1	1	3	-4	.010	.200	94.229	-2.	-2.	-.3
.1	276	2	1	3	-4	.010	.200	94.533	-1.	-1.	-.2
.0	277	1	0	3	-4	.010	.200	94.861	0.	0.	.0
.0	278	1	0	3	4	.010	.200	94.861	0.	0.	.0
.1	279	1	0	4	-3	.010	.200	95.100	-1.	-1.	.0
.1	280	1	0	4	3	.010	.200	95.100	-1.	-1.	.0
.0	281	2	0	3	-4	.010	.200	95.169	0.	0.	.0
.0	282	2	0	3	4	.010	.200	95.169	0.	0.	.0
.2	283	1	1	4	-3	.010	.200	95.288	-2.	-2.	-.3
.0	284	1	0	5	0	.010	.200	95.408	0.	0.	.0
.0	285	2	0	4	-3	.010	.200	95.409	0.	0.	.0

.0	286	2	0	4	3	.010	.200	95.409	0.	0.	.0	
.1	287	2	1	4	-3	.010	.200	95.597	-1.	-1.	-.2	
.0	288	1	1	1	-5	.010	.200	95.619	0.	0.	-.1	
.0	289	2	0	5	0	.010	.200	95.718	0.	0.	.0	
.0	290	2	1	1	-5	.010	.200	95.931	0.	0.	.0	
.0	291	1	3	2	3	.010	.200	96.084	0.	0.	.0	
.3	292	1	3	2	-4	.010	.200	96.254	-3.	-4.	-.5	
.0	293	2	3	2	3	.010	.200	96.398	0.	0.	.0	
.1	294	1	2	4	2	.010	.200	96.549	-1.	-1.	.0	
.0	295	1	3	4	0	.010	.200	96.568	0.	0.	.0	
.2	296	2	3	2	-4	.010	.200	96.569	-2.	-2.	-.1	
.1	297	1	3	4	-1	.010	.200	96.592	-2.	-1.	.1	
.0	298	1	4	3	-1	.010	.200	96.674	0.	0.	-.1	
.0	299	2	2	4	2	.010	.200	96.866	-1.	-1.	.0	
.0	300	2	3	4	0	.010	.200	96.885	0.	0.	.0	
	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
.1	301	2	3	4	-1	.010	.200	96.909	-1.	-1.	-.1	
.0	302	2	4	3	-1	.010	.200	96.991	0.	0.	.0	
.0	303	1	0	1	-5	.010	.200	97.075	0.	0.	.0	
.0	304	1	0	1	5	.010	.200	97.075	0.	0.	.0	
.0	305	2	0	1	-5	.010	.200	97.395	0.	0.	.0	
.0	306	2	0	1	5	.010	.200	97.395	0.	0.	.0	
.0	307	1	4	2	-3	.010	.200	97.398	0.	0.	.0	
.1	308	1	4	3	0	.010	.200	97.472	-1.	-1.	.1	
.0	309	2	4	2	-3	.010	.200	97.719	0.	0.	.0	
.1	310	2	4	3	0	.010	.200	97.794	-1.	-1.	-.1	
.1	311	1	0	5	-1	.010	.200	97.899	-1.	-1.	-.1	
.1	312	1	0	5	1	.010	.200	97.899	-1.	-1.	-.1	
.0	313	1	1	5	0	.010	.200	98.062	0.	0.	.0	
.1	314	2	0	5	-1	.010	.200	98.223	-1.	-1.	-.2	
.1	315	2	0	5	1	.010	.200	98.223	-1.	-1.	-.2	
.0	316	2	1	5	0	.010	.200	98.388	0.	0.	.0	
.1	317	1	5	0	0	.010	.200	98.637	-1.	-1.	-.2	

318	1	2	3	-4	.010	.200	98.903	0.	0.	.0
319	2	5	0	0	.010	.200	98.966	-1.	0.	.0
320	2	2	3	-4	.010	.200	99.233	0.	0.	.0
321	1	2	2	4	.010	.200	99.435	-1.	-2.	-.3
322	1	2	1	-5	.010	.200	99.479	0.	0.	.0
323	1	5	1	-1	.010	.200	99.548	0.	0.	.0
324	1	1	5	-1	.010	.200	99.740	-1.	-1.	-.2
325	2	2	2	4	.010	.200	99.769	-1.	-1.	-.1
326	2	2	1	-5	.010	.200	99.812	0.	0.	.0
327	2	5	1	-1	.010	.200	99.881	0.	0.	-.1

DERIVED BRAGG R-FACTOR= -5.9

NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
1	1	1	1	0	.305	.200	32.534	195.	182.	-13.1	
2	2	1	1	0	.306	.200	32.617	97.	90.	-7.1	
3	1	0	0	2	.328	.200	35.468	742.	689.	-53.1	
4	2	0	0	2	.329	.200	35.558	369.	340.	-29.2	
5	1	1	1	-1	.329	.200	35.559	2061.	1898.	-163.0	
6	2	1	1	-1	.330	.200	35.649	1025.	953.	-71.7	
7	1	1	1	1	.356	.200	38.754	2655.	2613.	-42.1	
8	2	1	1	1	.356	.200	38.853	1320.	1263.	-56.4	
9	1	2	0	0	.357	.200	38.968	566.	537.	-29.0	
10	2	2	0	0	.358	.200	39.067	282.	273.	-8.6	
11	1	1	1	-2	.421	.200	46.276	53.	48.	-5.2	
12	2	1	1	-2	.422	.200	46.396	27.	24.	-2.7	
13	1	2	0	-2	.444	.200	48.754	754.	764.	10.6	
14	2	2	0	-2	.445	.200	48.881	375.	412.	37.7	
15	1	1	1	2	.469	.200	51.403	35.	34.	-.4	
16	2	1	1	2	.471	.200	51.539	17.	16.	-.8	
17	1	0	2	0	.490	.200	53.503	271.	256.	-14.6	
18	2	0	2	0	.491	.200	53.646	135.	128.	-7.0	
19	1	0	2	-1	.522	.200	56.744	11.	10.	-.6	
20	1	0	2	1	.522	.200	56.744	11.	10.	-.6	
21	2	0	2	-1	.523	.200	56.896	5.	5.	-.2	
22	2	0	2	1	.523	.200	56.896	5.	5.	-.2	



.6	55	1	2	0	-4	.798	.200	80.213	47.	49.	2.2
.1	56	1	1	1	-4	.799	.200	80.317	5.	5.	.3
.3	57	2	2	0	-4	.801	.200	80.451	23.	25.	1.5
.0	58	2	1	1	-4	.802	.200	80.555	2.	3.	.2
1.4	59	1	3	1	-3	.828	.200	82.408	110.	129.	19.5
.7	60	2	3	1	-3	.832	.200	82.655	55.	65.	10.1
1.3	61	1	2	2	2	.839	.200	83.144	105.	121.	16.3
.7	62	2	2	2	2	.842	.200	83.395	52.	59.	6.7
.1	63	1	3	1	2	.845	.200	83.599	4.	5.	.5
1.2	64	1	4	0	0	.847	.200	83.684	94.	104.	9.7
.0	65	2	3	1	2	.849	.200	83.851	2.	2.	.2
.6	66	2	4	0	0	.850	.200	83.937	47.	51.	3.9
.4	67	1	4	0	-2	.890	.200	86.609	36.	38.	1.4
.0	68	1	2	2	-3	.893	.200	86.801	4.	4.	.1
.2	69	2	4	0	-2	.894	.200	86.875	18.	19.	.7
.0	70	2	2	2	-3	.897	.200	87.068	2.	2.	.1
.0	71	1	1	1	4	.913	.200	88.081	3.	4.	.2
.0	72	1	1	3	0	.913	.200	88.131	0.	0.	.0
.0	73	2	1	1	4	.917	.200	88.354	2.	2.	.1
.0	74	2	1	3	0	.918	.200	88.404	0.	0.	.0
1.8	75	1	1	3	-1	.940	.200	89.824	149.	161.	12.1
.9	76	2	1	3	-1	.945	.200	90.106	74.	80.	5.7
.7	77	1	1	3	1	.972	.200	91.754	61.	65.	3.8
.4	78	2	1	3	1	.977	.200	92.045	30.	32.	1.9
.3	79	1	2	0	4	1.040	.200	95.706	27.	31.	3.4
.2	80	2	2	0	4	1.046	.200	96.018	14.	15.	1.6
.0	81	1	1	3	-2	1.061	.200	96.850	0.	0.	.0
.0	82	2	1	3	-2	1.067	.200	97.168	0.	0.	.0
.0	83	1	3	1	-4	1.086	.200	98.169	3.	3.	.3
.0	84	1	2	2	3	1.090	.200	98.410	2.	3.	.3
.4	85	1	0	2	-4	1.091	.200	98.479	32.	36.	3.6
.4	86	1	0	2	4	1.091	.200	98.479	32.	36.	3.6
.0	87	2	3	1	-4	1.092	.200	98.495	1.	1.	.1



88	2	2	2	3	1.096	.200	98.737	1.	1.	.1
89	2	0	2	-4	1.098	.200	98.807	16.	18.	1.9
90	2	0	2	4	1.098	.200	98.807	16.	18.	1.9
91	1	3	1	3	1.118	.200	99.844	94.	110.	15.1

DERIVED BRAGG R-FACTOR= 8.4

## B. Perbandingan ZrO<sub>2</sub>-CuO 1 : 8

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**** MULTI-RIETVELD ANALYSIS PROGRAM LH-RIET 6.800
ZrCuO
NUMBER OF PHASES =      2
NUMBER OF HISTOGRAMS =    1
NUMBER OF PARAMETER LIMITS =    0
NUMBER OF BOND RESTRAINTS =    0

*** HISTOGRAM 1 ***
    FOR X-RAY DATA
    NEWTON-RAPHSON ALGORITHM
    BACKGROUND TO BE REFINED (MAX 6 PARAMETERS)
        - POLYNOMIAL BACKGROUND
    THE PSEDUO-VOIGT PROFILE FUNCTION WAS SELECTED
    - USING THE HOWARD, SUM OF 5 PEAKS, ASYMMETRY
    WAVELENGTHS = 1.54060 1.54439
    ALPHA2:ALPHA1 RATIO = .5000
    BASE OF PEAK = 2.0*HW* 7.00
    MONOCHROMATOR CORRECTION = 1.0000
    ABSORPTION CORRECTION FOR CYLINDER SAMPLE
    USING ALGORITHM OF SABINE(1996)/DWIGGINS(1972) WITH mu = .0000
    NO ILLUMINATION CORRECTION
    PREFERRED ORIENTATION USING MARCH MODEL - NO SUMMING OF EQUIVALENTS
    HISTOGRAM WEIGHTING = 1.0000
    NO OTHER GEOMETRY CORRECTIONS APPLIED

GENERATE OFF-LINE PLOT
    - ILL PLOT FILE OF OBS AND CALC DATA
OUTPUT STRUCTURE FACTORS
OUTPUT CORRELATION MATRIX
GENERATE NEW INPUT FILE
NUMBER OF CYCLES = 30
RELAXATION FACTORS:
    FOR COORDINATES, ISOTROPIC B, SITE OCCUPANCY = .90
    FOR ANISOTROPIC TEMPERATURE FACTORS = .90
    FOR SCALE, ZERO, B OVERALL, UNIT CELL, PREFERRED ORIENTATION BACKGROUND = .90
    FOR PEAK WIDTH, ASYMMETRY, SHAPE PARAMETERS = .90
EPS-VALUE = .100

NUMBER OF PARAMETERS VARIED = 29

GLOBAL PARAMETERS AND CODEWORDS:
    ZEROPOINT( 1) = .00 .00
HISTOGRAM READ IN AS (2THETA, INTENSITY)
HISTOGRAM 1 FROM 20.050000 TO 99.980000 IN STEPS OF .033000 DEGREES

    BACKGROUND PARAMETERS AND CODEWORDS( 1)
    396.300000 .000000 .000000 .000000 .000000 .000000
    11.000000 .000000 .000000 .000000 .000000 .000000

***** PHASE 1 *****
ZrO2

PHASE IS CALCULATED USING STRUCTURAL INPUT

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NUMBER OF FORMULA PER UNIT CELL = 1  
 NUMBER OF ATOMS = 3  
 PREFERRED ORIENTATION VECTOR( 1) = .0000 .0000 1.0000  
 THE SPACE GROUP IS P 21/C

\*\*\*INITIAL PARAMETERS\*\*\*

ATOM	NTP	X	Y	Z	B	N	B23
		B11	B22	B33	B12	B13	B23
ZR	ZR	.27582	.04112	.20822	1.00000	.25000	
		.00000	.00000	.00000	.00000	.00000	.00000
O	O	.07032	.33591	.34061	.00000	.50000	
		.00000	.00000	.00000	.00000	.00000	.00000
O	O	.44232	.75491	.47891	1.00000	.25000	
		.00000	.00000	.00000	.00000	.00000	.00000

\*\*\*\*\* PHASE INFORMATION \*\*\*\*\*

OVERALL SCALE FACTOR = .308841E-02  
 OVERALL TEMP. FACTOR = 2.12040  
 DIRECT CELL PARAMETERS = 5.1808 5.1495 5.2787 90.0120 99.6492 90.0009

\*\*\* HISTOGRAM 1 \*\*\*

HISTOGRAM SCALE FACTOR = 1.00000 .00  
 PREFERRED ORIENTATION PARAMETER = 1.0000  
 ABSORPTION R = .0000  
 ASYMMETRY PARAMETERS = .020000 .000000  
 GAUSSIAN HALF-WIDTH PARAMETERS = -2.9000 2.6000 -.2800  
 ANISOTROPIC PARAMETER = .000000  
 PSEUDO-VOIGT PEAK SHAPE =  
 .2000 + .00000 \* TWOTH + .000000 \* TWOTHSQ  
 EXTINCTION PARAMETER = .000000  
 The Laue symmetry is: 2/M

\*\*\*CODING OF VARIABLES\*\*\*

ATOM	X	Y	Z	B	N	B23
	B11	B22	B33	B12	B13	B23
ZR	.00	.00	.00	.00	.00	
	.00	.00	.00	.00	.00	.00
O	.00	.00	.00	.00	.00	
	.00	.00	.00	.00	.00	.00
O	.00	.00	.00	.00	.00	
	.00	.00	.00	.00	.00	.00

\*\*\*\*\* PHASE INFORMATION CODEWORDS \*\*\*\*\*

OVERALL SCALE FACTOR = 21.00  
 OVERALL TEMP. FACTOR = 31.00  
 CELL CONSTANTS = 71.00 81.00 91.00 101.00 111.00 121.00

\*\*\* HISTOGRAM 1 CODEWORDS \*\*\*

PREFERRED ORIENTATION PARAMETER = .00  
 ABSORPTION R/P<sub>0</sub> PARAMETER = .00  
 ASYMMETRY PARAMETERS = .00 .00  
 GAUSSIAN COMPONENT = 41.00 51.00 61.00  
 ANISOTROPIC = .00  
 LORENTZIAN COMPONENTS = 271.00 281.00 291.00  
 EXTINCTION = .00

FORMFACTORS FOR HISTOGRAM

FOR ZR DFP= -.314000 DFPP= 2.245000  
 COEFFICIENTS= 17.876500 1.276180 10.948000 11.916000 5.417320 .117622 3.657210  
 87.662700 2.069290  
 FOR O DFP= .047000 DFPP= .032000  
 COEFFICIENTS= 3.048500 13.277100 2.286800 5.701100 1.546300 .323900 .867000  
 32.908900 .250800  
 LAUE SYMMETRY 2/M WILL BE USED TO GENERATE INDICES

\*\*\*\*\* PHASE 2 \*\*\*\*\*

CuO

PHASE IS CALCULATED USING STRUCTURAL INPUT  
 NUMBER OF FORMULA PER UNIT CELL = 1  
 NUMBER OF ATOMS = 2  
 PREFERRED ORIENTATION VECTOR( 1) = .0000 .0000 1.0000  
 THE SPACE GROUP IS C 2/C

\*\*\*INITIAL PARAMETERS\*\*\*

ATOM	NTYP	X	Y	Z	B	N	B23
		B11	B22	B33	B12	B13	B23
CU	CU	.25000	.25000	.00000	.80000	.50000	.00000
		.00000	.00000	.00000	.00000	.00000	.00000
O	O	.00000	.41840	.25000	.70000	.50000	.00000
		.00000	.00000	.00000	.00000	.00000	.00000

\*\*\*\*\* PHASE INFORMATION \*\*\*\*\*

OVERALL SCALE FACTOR = .192015E-02  
 OVERALL TEMP. FACTOR = 1.11770  
 DIRECT CELL PARAMETERS = 4.6811 3.4224 5.1281 90.0314 99.4001 89.9652

\*\*\* HISTOGRAM 1 \*\*\*

HISTOGRAM SCALE FACTOR = 1.00000 .00  
 PREFERRED ORIENTATION PARAMETER = 1.0000  
 ABSORPTION R = .0000  
 ASYMMETRY PARAMETERS = .020000 .000000  
 GAUSSIAN HALF-WIDTH PARAMETERS = 2.7000 -2.3000 .5200  
 ANISOTROPIC PARAMETER = .000000  
 PSEUDO-VOIGT PEAK SHAPE =  
 -3.9641 + .19735 \* TWOTH + -.002020 \* TWOTHSQ  
 EXTINCTION PARAMETER = .000000  
 The Laue symmetry is: 2/M

\*\*\*CODING OF VARIABLES\*\*\*

ATOM	X	Y	Z	B	N	B23
	B11	B22	B33	B12	B13	B23
CU	.00	.00	.00	.00	.00	.00
	.00	.00	.00	.00	.00	.00
O	.00	.00	.00	.00	.00	.00
	.00	.00	.00	.00	.00	.00

\*\*\*\*\* PHASE INFORMATION CODEWORDS \*\*\*\*\*

OVERALL SCALE FACTOR = 131.00  
 OVERALL TEMP. FACTOR = 141.00  
 CELL CONSTANTS = 181.00 191.00 201.00 211.00 221.00 231.00

\*\*\* HISTOGRAM 1 CODEWORDS \*\*\*

PREFERRED ORIENTATION PARAMETER = .00  
 ABSORPTION R/po PARAMETER = .00  
 ASYMMETRY PARAMETERS = .00 .00  
 GAUSSIAN COMPONENT = 151.00 161.00 171.00  
 ANISOTROPIC = .00  
 LORENZTIAN COMPONENTS = 241.00 251.00 261.00  
 EXTINCTION = .00

FORMFACTORS FOR HISTOGRAM

FOR ZR DFP= -.314000 DFPP= 2.245000  
 COEFFICIENTS= 17.876500 1.276180 10.948000 11.916000 5.417320 .117622 3.657210  
 87.662700 2.069290  
 FOR O DFP= .047000 DFPP= .032000  
 COEFFICIENTS= 3.048500 13.277100 2.286800 5.701100 1.546300 .323900 .867000  
 32.908900 .250800  
 FOR CU DFP= -2.019000 DFPP= .589000  
 COEFFICIENTS= 13.338000 3.582800 7.167600 .247000 5.615800 11.396600 1.673500  
 64.812600 1.191000  
 LAUE SYMMETRY 2/M WILL BE USED TO GENERATE INDICES

+++++

CYCLE NUMBER= 1

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
ZR	.27582	.00000	.00000	.04112	.00000	.00000	.20822	.00000	.00000	
1.0000	.0000	.0000	.2500	.0000	.0000					
O	.07032	.00000	.00000	.33591	.00000	.00000	.34061	.00000	.00000	
.0000	.0000	.0000	.5000	.0000	.0000					
O	.44232	.00000	.00000	.75491	.00000	.00000	.47891	.00000	.00000	
1.0000	.0000	.0000	.2500	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

Phase: 1

PHASE SCALE FACTOR = .533885E-02 .225044E-02 .389524E-03  
OVERALL TEMP. FACTOR = 4.197104 2.076705 1.007608  
CELL PARAMETERS = 5.180871 .000071 .000218  
5.149547 .000047 .000281  
5.278597 -.000103 .000163  
89.998500 -.013496 .004147  
99.650830 .001633 .003710  
89.999830 -.001068 .006115  
RECIPROCAL CELL = .196 .194 .192 90.002 80.349 90.000  
CELL VOLUME = 138.835400 .098471  
SCALE \* VOLUME = .741221 .054082  
MOLECULAR WEIGHT = 139.220  
DENSITY = 1.664

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = 35674.9

Histogram: 1

SCALE FACTOR = 1.0000 .00000 .00000  
ZEROPOINT = .00000 .00000 .00000

BACKGROUND PARAMETER B 0 = 389.343 -6.95720 2.50229  
PREFERRED ORIENTATION = 1.00000 .00000 .00000  
ABSORPTION R = .00000 .00000 .00000  
ASYMMETRY PARAMETERS = .02000 .00000 .00000

			.00000	.00000	.00000	
HALFWIDTH PARAMETERS U	=		-2.904695	-.004695	.003592	
	V	=	2.608981	.008981	.007110	
	W	=	-.284227	-.004227	.003497	
ANISOTROPIC GAUSSIAN BROADENING	=		.000000	.000000	.000000	
PEAK SHAPE PARAMETER Gam0	=	7.462652	7.262652	1.312841		
PEAK SHAPE PARAMETER Gam1	=	-.246256	-.246256	.059767		
PEAK SHAPE PARAMETER Gam2	=	.002036	.002036	.000581		
EXTINCTION PARAMETER	=	.000000	.000000	.000000		

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
.8000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
.7000	.0000	.0000	.5000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

```

+-----+
|                               |
|                               |
+-----+

```

PHASE SCALE FACTOR	=	.176815E-02	-.152002E-03	.114891E-03
OVERALL TEMP. FACTOR	=	.302475	-.815225	.591519
CELL PARAMETERS	=	4.681254	.000154	.001435
		3.422414	.000014	.001424
		5.128511	.000411	.001655
		90.028370	-.003029	.022862
		99.396650	-.003448	.024537
		89.978220	.013016	.037181
RECIPROCAL CELL	=	.217	.292	.198
CELL VOLUME	=	81.062320	.310648	
SCALE * VOLUME	=	.143330	.009330	
MOLECULAR WEIGHT	=	318.200		
DENSITY	=	6.515		

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = 15767.1

```

+-----+
|                               |
|                               |
+-----+

```

SCALE FACTOR	=	1.0000	.00000	.00000
ZEROPOINT	=	.00000	.00000	.00000

BACKGROUND PARAMETER B 0	=	389.343	-6.95720	2.50229
PREFERRED ORIENTATION	=	1.00000	.00000	.00000
ABSORPTION R	=	.00000	.00000	.00000
ASYMMETRY PARAMETERS	=	.02000	.00000	.00000
		.00000	.00000	.00000

HALFWIDTH PARAMETERS U	=	2.673293	-.026707	.154818
V	=	-2.267449	.032551	.203976
W	=	.522151	.002151	.053907
ANISOTROPIC GAUSSIAN BROADENING	=	.000000	.000000	.000000
PEAK SHAPE PARAMETER Gam0	=	-4.562980	-.598880	1.439323
PEAK SHAPE PARAMETER Gam1	=	.215837	.018487	.060820
PEAK SHAPE PARAMETER Gam2	=	-.002094	-.000074	.000612
EXTINCTION PARAMETER	=	.000000	.000000	.000000

MOLAR PERCENTAGE OF PHASES:	WEIGHT PERCENTAGE OF PHASES:
PHASE 1: 83.80 8.03	69.35 6.31
PHASE 2: 16.20 1.46	30.65 2.60

Hist	Rp	Rwp	Rexp	Durbin Unwght	Durbin Wght	N-P
1	9.40	15.10	4.69	.126	.186	2394
SUMYDIF	SUMYOBS	SUMYCALC	SUMWYOBSSQ	GOF	CONDITION	
.1024E+06	.1090E+07	.1069E+07	.1090E+07	.1038E+02	.8206E+13	

+++++

CYCLE NUMBER= 2

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
ZR	.27582	.00000	.00000	.04112	.00000	.00000	.20822	.00000	.00000	
1.0000	.0000	.0000	.2500	.0000	.0000					
O	.07032	.00000	.00000	.33591	.00000	.00000	.34061	.00000	.00000	
.0000	.0000	.0000	.5000	.0000	.0000					
O	.44232	.00000	.00000	.75491	.00000	.00000	.47891	.00000	.00000	
1.0000	.0000	.0000	.2500	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

Phase: 1
----------

PHASE SCALE FACTOR	=	.492850E-02	-.410350E-03	.457138E-03
OVERALL TEMP. FACTOR	=	1.367026	-2.830078	1.009265
CELL PARAMETERS	=	5.180781	-.000090	.000595
		5.149514	-.000033	.000425
		5.278802	.000205	.000533
		89.989110	-.009399	.011538
		99.660010	.009178	.013208
		90.002560	.002731	.013592

PHASE SCALE FACTOR	=	.179803E-02	.298840E-04	.968314E-04		
OVERALL TEMP. FACTOR	=	.416443	.113968	.514096		
CELL PARAMETERS	=	4.681111	-.000143	.001610		
		3.422517	.000103	.001604		
		5.128592	.000082	.001897		
		90.030620	.002243	.026143		
		99.396840	.000191	.028414		
		89.974800	-.003418	.041917		
RECIPROCAL CELL	=	.217	.292	.198	89.973	80.603 90.020

ABSOLUTE PHASE VALUES:

MASS = MASS OF PHASE IN BEAM (in g)

$$l_s/R = \text{RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR}$$

Then :

$$\text{INC} \cdot \text{MASS} \cdot l_s / R = 16033.8$$

Histogram: 1

```
SCALE FACTOR      = 1.0000      .00000      .00000
ZEROPOINT         =      .00000      .00000      .00000
```

BACKGROUND PARAMETER B 0	=	386.181	-3.16225	2.32694
PREFERRED ORIENTATION	=	1.00000	.00000	.00000
ABSORPTION R	=	.00000	.00000	.00000
ASYMMETRY PARAMETERS	=	.02000	.00000	.00000
		.00000	.00000	.00000
HALFWIDTH PARAMETERS U	=	2.694416	.021123	.150602
V	=	-2.294502	-.027053	.191842
W	=	.530984	.008833	.050064
ANISOTROPIC GAUSSIAN BROADENING	=	.000000	.000000	.000000
PEAK SHAPE PARAMETER Gam0	=	-4.271573	.291407	1.246112
PEAK SHAPE PARAMETER Gam1	=	.205190	-.010647	.052730
PEAK SHAPE PARAMETER Gam2	=	-.002011	.000083	.000531
EXTINCTION PARAMETER	=	.000000	.000000	.000000

MOLAR PERCENTAGE OF PHASES:				WEIGHT PERCENTAGE OF PHASES:	
PHASE 1:	82.44	9.94	67.26	7.61	
PHASE 2:	17.56	1.65	32.74	2.76	

Hist	Rp	Rwp	Rexp	Durbin Unwght	Durbin Wght	N-P
1	9.05	14.98	4.69	.115	.167	2394

SUMYDIF	SUMYOBS	SUMYCALC	SUMWYOBSQ	GOF	CONDITION
.9858E+05	.1090E+07	.1064E+07	.1090E+07	.1022E+02	.1056E+13

CYCLE NUMBER= 3

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

DB	SB	N	DN	SN						
ZR	.27582	.00000	.00000	.04112	.00000	.00000	.20822	.00000	.00000	
.0000	.0000	.0000	.2500	.0000	.0000					
O	.07032	.00000	.00000	.33591	.00000	.00000	.34061	.00000	.00000	
.0000	.0000	.0000	.5000	.0000	.0000					
O	.44232	.00000	.00000	.75491	.00000	.00000	.47891	.00000	.00000	
.0000	.0000	.0000	.2500	.0000	.0000					

ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33
SB33	B12	DB12	SB12	B13	DB13	SB13	B23	DB23

SB23



ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								

```

+-----+
|               Phase: 1               |
+-----+

```

```

PHASE SCALE FACTOR   = .540358E-02 .475077E-03 .355521E-03
OVERALL TEMP. FACTOR = 2.954026 1.587000 .515019
CELL PARAMETERS      = 5.180724 -.000057 .000211
                      5.149444 -.000070 .000158
                      5.278800 -.000002 .000145
                      89.987930 -.001175 .002523
                      99.659140 -.000870 .002312
                      90.000300 -.002266 .004885
RECIPROCAL CELL      = .196 .194 .192 90.012 80.341 90.002
CELL VOLUME          = 138.830600 .060145
SCALE * VOLUME       = .750182 .049358
MOLECULAR WEIGHT     = 139.220
DENSITY              = 1.664

```

ABSOLUTE PHASE VALUES:

```

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
MASS = MASS OF PHASE IN BEAM (in g)
ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

```

Then:

INC\*MASS\*ls/R = 36106.2

```

+-----+
|               Histogram: 1             |
+-----+

```

```

SCALE FACTOR          = 1.0000 .00000 .00000
ZEROPOINT             = .00000 .00000 .00000

BACKGROUND PARAMETER B 0 = 388.140 1.95980 2.45157
PREFERRED ORIENTATION   = 1.00000 .00000 .00000
ABSORPTION R           = .00000 .00000 .00000
ASYMMETRY PARAMETERS   = .02000 .00000 .00000
                      .00000 .00000 .00000
HALFWIDTH PARAMETERS U = -2.922108 -.003502 .003995
                      V = 2.644237 .007177 .007931
                      W = -.301501 -.003621 .003847
ANISOTROPIC GAUSSIAN BROADENING = .000000 .000000 .000000
PEAK SHAPE PARAMETER Gam0 = 4.669996 .823098 .712678
PEAK SHAPE PARAMETER Gam1 = -.148597 -.039877 .033020
PEAK SHAPE PARAMETER Gam2 = .001267 .000363 .000304
EXTINCTION PARAMETER   = .000000 .000000 .000000

```

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
.8000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
.7000	.0000	.0000	.5000	.0000	.0000					

ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33
SB33								
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23
SB23								
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								

```

+-----+
|                               |
|           Phase:  2         |
|                               |
+-----+

```

```

PHASE SCALE FACTOR   = .178006E-02-.179694E-04 .995272E-04
OVERALL TEMP. FACTOR = .345718 -.070725 .531352
CELL PARAMETERS      =  4.681012  -.000099  .001605
                      3.422555  .000039  .001566
                      5.128582  -.000011  .001903
                      90.029210  -.001411  .025866
                      99.397470  .000626  .027769
                      89.974430  -.000366  .041045
RECIPROCAL CELL      =  .217  .292  .198  89.975  80.603  90.021
CELL VOLUME          =  81.062390  .351397
SCALE * VOLUME       =  .144296  .008092
MOLECULAR WEIGHT     =  318.200
DENSITY              =  6.515

```

#### ABSOLUTE PHASE VALUES:

```

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
MASS = MASS OF PHASE IN BEAM (in g)
ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

```

Then:

INC\*MASS\*ls/R = 15873.3

```

+-----+
|                               |
|           Histogram:  1         |
|                               |
+-----+

```

```

SCALE FACTOR          = 1.0000  .00000  .00000
ZEROPOINT             = .00000  .00000  .00000

BACKGROUND PARAMETER B 0 = 388.140  1.95980  2.45157
PREFERRED ORIENTATION   = 1.00000  .00000  .00000
ABSORPTION R           = .00000  .00000  .00000
ASYMMETRY PARAMETERS   = .02000  .00000  .00000
                      .00000  .00000  .00000
HALFWIDTH PARAMETERS U = 2.633050  -.061366  .170459
                      V = -2.199910  .094592  .227683
                      W = .506890  -.024094  .059958
ANISOTROPIC GAUSSIAN BROADENING = .000000  .000000  .000000
PEAK SHAPE PARAMETER Gam0 = -3.967838  .303734  1.273768
PEAK SHAPE PARAMETER Gam1 = .192120  -.013070  .053490
PEAK SHAPE PARAMETER Gam2 = -.001892  .000119  .000532
EXTINCTION PARAMETER   = .000000  .000000  .000000

```

#### MOLAR PERCENTAGE OF PHASES:

```

PHASE 1:  83.87  7.24
PHASE 2:  16.13  1.28

```

#### WEIGHT PERCENTAGE OF PHASES:

```

69.46  5.69
30.54  2.27

```

```

+-----+
| Hist | Rp | Rwp | Rexp | Durbin Unwght | Durbin Wght | N-P |
+-----+
| 1 | 9.14 | 14.80 | 4.69 | .136 | .206 | 2394 |
+-----+
| SUMYDIF | SUMYOBS | SUMYCALC | SUMWYOBSQ | GOF | CONDITION |
+-----+

```

```

| .9957E+05| .1090E+07| .1070E+07| .1090E+07| .9968E+01| .8417E+13|
+-----+
+++++
+++++
CYCLE NUMBER= 4

PHASE 1: ZrO2
NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM      X      DX      SX      Y      DY      SY      Z      DZ      SZ      B
DB SB      N      DN      SN
ZR      .27582 .00000 .00000 .04112 .00000 .00000 .20822 .00000 .00000
1.0000 .0000 .0000 .2500 .0000 .0000
O      .07032 .00000 .00000 .33591 .00000 .00000 .34061 .00000 .00000
.0000 .0000 .0000 .5000 .0000 .0000
O      .44232 .00000 .00000 .75491 .00000 .00000 .47891 .00000 .00000
1.0000 .0000 .0000 .2500 .0000 .0000
ATOM      B11      DB11      SB11      B22      DB22      SB22      B33      DB33
SB33
      B12      DB12      SB12      B13      DB13      SB13      B23      DB23
SB23
ZR      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
O      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
O      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000

+-----+
| Phase: 1 |
+-----+
PHASE SCALE FACTOR = .520054E-02-.203043E-03 .408106E-03
OVERALL TEMP. FACTOR = 2.562267 -.391759 .756028
CELL PARAMETERS = 5.180675 -.000049 .000381
                  5.149384 -.000061 .000207
                  5.278822 .000022 .000257
                  89.986020 -.001907 .004912
                  99.656090 -.003052 .005427
                  89.999370 -.000923 .008001
RECIPROCAL CELL = .196 .194 .192 90.014 80.344 90.003
CELL VOLUME = 138.829500 .116813
SCALE * VOLUME = .721987 .056660
MOLECULAR WEIGHT = 139.220
DENSITY = 1.664
ABSOLUTE PHASE VALUES:
  INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
  MASS = MASS OF PHASE IN BEAM (in g)
  ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR
Then:
  INC*MASS*ls/R = 34749.2

+-----+
| Histogram: 1 |
+-----+
SCALE FACTOR = 1.0000 .00000 .00000
ZEROPOINT = .00000 .00000 .00000

BACKGROUND PARAMETER B 0 = 388.300 .160086 2.52259
PREFERRED ORIENTATION = 1.00000 .00000 .00000
ABSORPTION R = .00000 .00000 .00000
ASYMMETRY PARAMETERS = .02000 .00000 .00000

```

			.00000	.00000	.00000	
HALFWIDTH PARAMETERS U	=		-2.930523	-.008415	.006636	
V	=		2.661674	.017437	.013154	
W	=		-.310318	-.008816	.006340	
ANISOTROPIC GAUSSIAN BROADENING	=		.000000	.000000	.000000	
PEAK SHAPE PARAMETER Gam0	=	4.607166	-.062829	.859441		
PEAK SHAPE PARAMETER Gam1	=	-.147438	.001159	.040936		
PEAK SHAPE PARAMETER Gam2	=	.001290	.000023	.000398		
EXTINCTION PARAMETER	=	.000000	.000000	.000000		

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
.8000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
.7000	.0000	.0000	.5000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

```

+-----+
|                               |
|                               |
+-----+

```

PHASE SCALE FACTOR	=	.180287E-02	.228067E-04	.986283E-04
OVERALL TEMP. FACTOR	=	.496750	.151032	.535939
CELL PARAMETERS	=	4.680833	-.000178	.001611
		3.422380	-.000175	.001582
		5.128878	.000297	.001917
		90.027600	-.001610	.026080
		99.397360	-.000107	.028148
		89.972520	-.001915	.041361
RECIPROCAL CELL	=	.217	.292	.198
CELL VOLUME	=	81.059880	.354289	
SCALE * VOLUME	=	.146140	.008020	
MOLECULAR WEIGHT	=	318.200		
DENSITY	=	6.516		

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = 16076.2

```

+-----+
|                               |
|                               |
+-----+

```

SCALE FACTOR	=	1.0000	.00000	.00000
ZEROPOINT	=	.00000	.00000	.00000

BACKGROUND PARAMETER B 0	=	388.300	.160086	2.52259
PREFERRED ORIENTATION	=	1.00000	.00000	.00000
ABSORPTION R	=	.00000	.00000	.00000
ASYMMETRY PARAMETERS	=	.02000	.00000	.00000
		.00000	.00000	.00000

```

HALFWIDTH PARAMETERS U      =      2.565694      -.067355      .182008
                        V      =      -2.077846      .122064      .246512
                        W      =      .472515      -.034375      .064825
ANISOTROPIC GAUSSIAN BROADENING =      .000000      .000000      .000000
PEAK SHAPE PARAMETER  Gam0   =    -3.527252    .440586    1.244491
PEAK SHAPE PARAMETER  Gam1   =      .176154    -.015966    .052044
PEAK SHAPE PARAMETER  Gam2   =     -.001780    .000112    .000516
EXTINCTION PARAMETER   =      .000000    .000000    .000000

```

```

MOLAR PERCENTAGE OF PHASES:      WEIGHT PERCENTAGE OF PHASES:
PHASE  1:      83.17      8.52      68.37      6.61
PHASE  2:      16.83      1.44      31.63      2.49

```

```

+-----+
| Hist |   Rp |   Rwp |   Rexp | Durbin Unwght | Durbin Wght |   N-P |
+-----+
|    1 |  9.06 | 14.69 |  4.69 |      .124 |      .180 | 2394 |
+-----+
| SUMYDIF | SUMYOBS | SUMYCALC | SUMWYOBSSQ |   GOF   | CONDITION |
+-----+
| .9873E+05 | .1090E+07 | .1069E+07 | .1090E+07 | .9828E+01 | .2833E+13 |
+-----+

```

```

+++++
+++++

```

CYCLE NUMBER= 5

PHASE 1: ZrO2

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
ZR	.27582	.00000	.00000	.04112	.00000	.00000	.20822	.00000	.00000	
1.0000	.0000	.0000	.2500	.0000	.0000					
O	.07032	.00000	.00000	.33591	.00000	.00000	.34061	.00000	.00000	
.0000	.0000	.0000	.5000	.0000	.0000					
O	.44232	.00000	.00000	.75491	.00000	.00000	.47891	.00000	.00000	
1.0000	.0000	.0000	.2500	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

```

+-----+
| Phase: 1 |
+-----+

```

```

PHASE SCALE FACTOR = .515455E-02-.459871E-04 .395871E-03
OVERALL TEMP. FACTOR = 2.442656 -.119611 .731121
CELL PARAMETERS =
                    5.180540 -.000135 .000368
                    5.149426 .000042 .000167
                    5.278655 -.000167 .000305
                    89.984830 -.001190 .006157
                    99.654280 -.001808 .007549
                    89.998680 -.000694 .007577

```

ABSOLUTE PHASE VALUES:

MASS = MASS OF PHASE IN BEAM (in g)

Then:

$$\text{INC} \cdot \text{MASS} \cdot l_s / R = 34440.4$$

```
SCALE FACTOR      = 1.0000      .00000      .00000
ZEROPOINT         =      .00000      .00000      .00000
```

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

Phase: 2
----------

PHASE SCALE FACTOR	=	.179333E-02	-.954366E-05	.102839E-03		
OVERALL TEMP. FACTOR	=	.439987	-.056763	.558737		
CELL PARAMETERS	=	4.680844	.000011	.001616		
		3.422358	-.000023	.001616		
		5.128841	-.000037	.001904		
		90.028030	.000435	.026373		
		99.397140	-.000221	.028695		
		89.971600	-.000916	.042047		
RECIPROCAL CELL	=	.217	.292	.198	89.976	80.603 90.024



ZR	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000								

```

+-----+
|                               |
|           Phase:  1         |
|                               |
+-----+

```

```

PHASE SCALE FACTOR   = .520165E-02 .470983E-04 .387637E-03
OVERALL TEMP. FACTOR =  2.725752  .283096  .697973
CELL PARAMETERS      =   5.180714   .000175   .000298
                      5.149421  -.000004   .000162
                      5.278716   .000061   .000319
                      89.983180  -.001648   .005211
                      99.655360   .001083   .005319
                      89.999620   .000938   .007196
RECIPROCAL CELL      =   .196   .194   .192  90.017  80.345  90.003
CELL VOLUME          =  138.829000  .123691
SCALE * VOLUME       =   .722140   .053819
MOLECULAR WEIGHT     =   139.220
DENSITY              =   1.664

```

ABSOLUTE PHASE VALUES:

```

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
MASS = MASS OF PHASE IN BEAM (in g)
ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

```

Then:

INC\*MASS\*ls/R = 34756.5

```

+-----+
|                               |
|           Histogram: 1       |
|                               |
+-----+

```

```

SCALE FACTOR          = 1.0000   .00000   .00000
ZEROPOINT             =   .00000   .00000   .00000

BACKGROUND PARAMETER B 0 =   388.582   .372501   2.50060
PREFERRED ORIENTATION   =   1.00000   .00000   .00000
ABSORPTION R           =   .00000   .00000   .00000
ASYMMETRY PARAMETERS   =   .02000   .00000   .00000
                      .00000   .00000   .00000
HALFWIDTH PARAMETERS U =   -2.954992   -.011001   .006849
                      V   =   2.711383   .022343   .013612
                      W   =   -.335089   -.011147   .006666
ANISOTROPIC GAUSSIAN BROADENING =   .000000   .000000   .000000
PEAK SHAPE PARAMETER Gam0 =   4.695368   .184107   .788905
PEAK SHAPE PARAMETER Gam1 =   -.149799   -.008261   .036451
PEAK SHAPE PARAMETER Gam2 =   .001289   .000071   .000324
EXTINCTION PARAMETER   =   .000000   .000000   .000000

```

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
.8000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
.7000	.0000	.0000	.5000	.0000	.0000					



ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33
SB33								
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23
SB23								
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000
.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000

```

+-----+
|                               |
|           Phase:  2         |
|                               |
+-----+

```

```

PHASE SCALE FACTOR   = .178673E-02-.659433E-05 .102437E-03
OVERALL TEMP. FACTOR = .397807 -.042180 .560334
CELL PARAMETERS      =  4.680809  -.000036  .001632
                      3.422284  -.000073  .001648
                      5.128776  -.000066  .001928
                      90.028180  .000145  .026692
                      99.397710  .000572  .029191
                      89.968890  -.002716  .042775
RECIPROCAL CELL      =  .217   .292   .198  89.977  80.602  90.027
CELL VOLUME          =  81.055470  .362595
SCALE * VOLUME       =  .144824  .008328
MOLECULAR WEIGHT     =  318.200
DENSITY              =  6.516

```

ABSOLUTE PHASE VALUES:

```

INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
MASS = MASS OF PHASE IN BEAM (in g)
ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

```

Then:

INC\*MASS\*ls/R = 15931.4

```

+-----+
|                               |
|           Histogram:  1         |
|                               |
+-----+

```

```

SCALE FACTOR          = 1.0000  .00000  .00000
ZEROPOINT             = .00000  .00000  .00000

BACKGROUND PARAMETER B 0 = 388.582  .372501  2.50060
PREFERRED ORIENTATION   = 1.00000  .00000  .00000
ABSORPTION R           = .00000  .00000  .00000
ASYMMETRY PARAMETERS   = .02000  .00000  .00000
                      .00000  .00000  .00000
HALFWIDTH PARAMETERS U = 2.552349  -.005547  .192862
                      V = -2.005472  .034449  .260001
                      W = .449323  -.010997  .068048
ANISOTROPIC GAUSSIAN BROADENING = .000000  .000000  .000000
PEAK SHAPE PARAMETER Gam0 = -3.089407  .277046  1.247585
PEAK SHAPE PARAMETER Gam1 = .157826  -.011655  .052294
PEAK SHAPE PARAMETER Gam2 = -.001604  .000112  .000524
EXTINCTION PARAMETER   = .000000  .000000  .000000

```

MOLAR PERCENTAGE OF PHASES:

```

PHASE 1:  83.30  8.12
PHASE 2:  16.70  1.42

```

WEIGHT PERCENTAGE OF PHASES:

```

68.57  6.32
31.43  2.48

```

```

+-----+
| Hist | Rp | Rwp | Rexp | Durbin Unwght | Durbin Wght | N-P |
+-----+
| 1 | 9.07 | 14.71 | 4.69 | .125 | .182 | 2394 |
+-----+
| SUMYDIF | SUMYOBS | SUMYCALC | SUMWYOBSQ | GOF | CONDITION |
+-----+

```

```

| .9889E+05| .1090E+07| .1069E+07| .1090E+07| .9854E+01| .4356E+13|
+-----+
+++++
+++++
CYCLE NUMBER= 7

PHASE 1: ZrO2
NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM      X      DX      SX      Y      DY      SY      Z      DZ      SZ      B
DB SB      N      DN      SN
ZR      .27582 .00000 .00000 .04112 .00000 .00000 .20822 .00000 .00000
1.0000 .0000 .0000 .2500 .0000 .0000
O      .07032 .00000 .00000 .33591 .00000 .00000 .34061 .00000 .00000
.0000 .0000 .0000 .5000 .0000 .0000
O      .44232 .00000 .00000 .75491 .00000 .00000 .47891 .00000 .00000
1.0000 .0000 .0000 .2500 .0000 .0000
ATOM      B11      DB11      SB11      B22      DB22      SB22      B33      DB33
SB33
      B12      DB12      SB12      B13      DB13      SB13      B23      DB23
SB23
ZR      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
O      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
O      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000
      .000000 .000000 .000000 .000000 .000000 .000000 .000000 .000000
.000000

+-----+
| Phase: 1 |
+-----+
PHASE SCALE FACTOR = .513478E-02-.668631E-04 .393202E-03
OVERALL TEMP. FACTOR = 2.656146 -.069606 .734611
CELL PARAMETERS = 5.180678 -.000036 .000436
                  5.149428 .000007 .000161
                  5.278475 -.000241 .000341
                  89.986570 .003387 .005637
                  99.653660 -.001709 .006472
                  89.999690 .000069 .009193
RECIPROCAL CELL = .196 .194 .192 90.014 80.346 90.003
CELL VOLUME = 138.822600 .133985
SCALE * VOLUME = .712824 .054590
MOLECULAR WEIGHT = 139.220
DENSITY = 1.665
ABSOLUTE PHASE VALUES:
  INC = NEUTRONS ON SAMPLE/CM^2 ( in cm^-2)
  MASS = MASS OF PHASE IN BEAM (in g)
  ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR
Then:
  INC*MASS*ls/R = 34308.1

+-----+
| Histogram: 1 |
+-----+
SCALE FACTOR = 1.0000 .00000 .00000
ZEROPOINT = .00000 .00000 .00000

BACKGROUND PARAMETER B 0 = 388.602 .194495E-01 2.50243
PREFERRED ORIENTATION = 1.00000 .00000 .00000
ABSORPTION R = .00000 .00000 .00000
ASYMMETRY PARAMETERS = .02000 .00000 .00000

```

			.00000	.00000	.00000	
HALFWIDTH PARAMETERS U	=		-2.967721	-.012729	.007074	
V	=		2.737170	.025786	.014021	
W	=		-.347869	-.012780	.006846	
ANISOTROPIC GAUSSIAN BROADENING	=		.000000	.000000	.000000	
PEAK SHAPE PARAMETER Gam0	=	4.663916	-.031452	.835994		
PEAK SHAPE PARAMETER Gam1	=	-.146887	.002912	.039120		
PEAK SHAPE PARAMETER Gam2	=	.001240	-.000049	.000361		
EXTINCTION PARAMETER	=	.000000	.000000	.000000		

PHASE 2: CuO

NEW PARAMETERS, SHIFTS, AND STANDARD DEVIATIONS=

ATOM	X	DX	SX	Y	DY	SY	Z	DZ	SZ	B
DB	SB	N	DN	SN						
CU	.25000	.00000	.00000	.25000	.00000	.00000	.00000	.00000	.00000	
.8000	.0000	.0000	.5000	.0000	.0000					
O	.00000	.00000	.00000	.41840	.00000	.00000	.25000	.00000	.00000	
.7000	.0000	.0000	.5000	.0000	.0000					
ATOM	B11	DB11	SB11	B22	DB22	SB22	B33	DB33		
SB33										
	B12	DB12	SB12	B13	DB13	SB13	B23	DB23		
SB23										
CU	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
O	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										
	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	.000000	
.000000										

```

+-----+
|                               |
|                               |
+-----+

```

PHASE SCALE FACTOR	=	.178533E-02	-.139745E-05	.102171E-03
OVERALL TEMP. FACTOR	=	.387569	-.010238	.561902
CELL PARAMETERS	=	4.680710	-.000098	.001643
		3.422181	-.000103	.001675
		5.128879	.000103	.001952
		90.028050	-.000122	.026900
		99.397510	-.000198	.029514
		89.966990	-.001900	.043388
RECIPROCAL CELL	=	.217	.292	.198
CELL VOLUME	=	81.052990	.365447	
SCALE * VOLUME	=	.144707	.008307	
MOLECULAR WEIGHT	=	318.200		
DENSITY	=	6.516		

ABSOLUTE PHASE VALUES:

INC = NEUTRONS ON SAMPLE/CM<sup>2</sup> ( in cm<sup>-2</sup>)

MASS = MASS OF PHASE IN BEAM (in g)

ls/R = RATIO OF DETECTOR HEIGHT TO SAMPLE-DETECTOR

Then:

INC\*MASS\*ls/R = 15918.5

```

+-----+
|                               |
|                               |
+-----+

```

SCALE FACTOR	=	1.0000	.00000	.00000
ZEROPOINT	=	.00000	.00000	.00000

BACKGROUND PARAMETER B 0	=	388.602	.194495E-01	2.50243
PREFERRED ORIENTATION	=	1.00000	.00000	.00000
ABSORPTION R	=	.00000	.00000	.00000
ASYMMETRY PARAMETERS	=	.02000	.00000	.00000
		.00000	.00000	.00000

HALFWIDTH PARAMETERS U	=	2.540752	-.011597	.203500
V	=	-1.956988	.048484	.274182
W	=	.433958	-.015364	.071599
ANISOTROPIC GAUSSIAN BROADENING	=	.000000	.000000	.000000
PEAK SHAPE PARAMETER Gam0	=	-2.792790	.296617	1.247697
PEAK SHAPE PARAMETER Gam1	=	.145911	-.011915	.052111
PEAK SHAPE PARAMETER Gam2	=	-.001497	.000107	.000519
EXTINCTION PARAMETER	=	.000000	.000000	.000000

MOLAR PERCENTAGE OF PHASES:	WEIGHT PERCENTAGE OF PHASES:
PHASE 1: 83.13 8.32	68.31 6.46
PHASE 2: 16.87 1.46	31.69 2.53

Hist	Rp	Rwp	Rexp	Durbin Unwght	Durbin Wght	N-P
1	9.07	14.71	4.69	.124	.180	2394
SUMYDIF	SUMYOBS	SUMYCALC	SUMWYOBSSQ	GOF	CONDITION	
.9883E+05	.1090E+07	.1069E+07	.1090E+07	.9849E+01	.3628E+13	

CORRELATION MATRIX=

	1	2	3	4	5	6	7	8	9	10	11	12	13
14	15	16	17	18	19								
1	100	-32	24	1	0	2	6	5	-1	-1	1	-4	25
42	-1	9	-9	6	0								
2	-32	100	63	15	-15	16	0	0	-2	-1	1	0	-25
-29	0	-2	4	-1	0								
3	24	63	100	23	-24	26	5	2	-4	-3	3	-3	-15
-16	-2	2	0	-1	-1								
4	1	15	23	100	-99	99	-37	-29	14	14	8	34	-2
-4	-1	2	0	0	0								
5	0	-15	-24	-99	100	-99	39	31	-13	-14	-7	-33	4
5	3	-1	1	1	0								
6	2	16	26	99	-99	100	-38	-31	14	16	8	35	-3
-4	-2	2	0	0	0								
7	6	0	5	-37	39	-38	100	24	-6	-31	11	-79	0
0	3	-1	2	0	0								
8	5	0	2	-29	31	-31	24	100	-17	22	-26	-27	0
1	2	-1	2	0	1								
9	-1	-2	-4	14	-13	14	-6	-17	100	20	19	-10	0
0	3	-2	3	0	0								
10	-1	-1	-3	14	-14	16	-31	22	20	100	-51	24	1
1	0	1	0	1	0								
11	1	1	3	8	-7	8	11	-26	19	-51	100	5	0
0	0	1	0	0	-1								
12	-4	0	-3	34	-33	35	-79	-27	-10	24	5	100	0
0	-3	3	-2	1	0								
13	25	-25	-15	-2	4	-3	0	0	0	1	0	0	100
91	-1	6	-8	-3	-2								
14	42	-29	-16	-4	5	-4	0	1	0	1	0	0	91
100	-2	8	-9	2	-2								
15	-1	0	-2	-1	3	-2	3	2	3	0	0	-3	-1
-2	100	-98	97	-8	-1								
16	9	-2	2	2	-1	2	-1	-1	-2	1	1	3	6
8	-98	100	-98	10	2								
17	-9	4	0	0	1	0	2	2	3	0	0	-2	-8
-9	97	-98	100	-9	-2								
18	6	-1	-1	0	1	0	0	0	0	1	0	1	-3
2	-8	10	-9	100	19								
19	0	0	-1	0	0	0	0	1	0	0	-1	0	-2
-2	-1	2	-2	19	100								
20	-2	4	5	2	-1	2	1	1	0	0	0	-1	-6
-10	19	-20	25	-28	-23								





29	1	2	1	0	.507	.796	39.351	238.	239.	.9		
1.7	30	2	2	1	0	.507	.791	39.452	119.	121.	2.4	
.9	31	1	1	1	-2	.511	.758	40.149	1.	1.	.1	
.0	32	2	1	1	-2	.512	.754	40.252	0.	0.	.1	
.0	33	1	2	1	-1	.513	.738	40.590	961.	1377.	416.3	
9.7	34	2	2	1	-1	.514	.733	40.694	478.	676.	198.6	
4.7	35	1	1	0	2	.518	.699	41.473	300.	287.	-13.3	
2.3	36	2	1	0	2	.518	.695	41.580	149.	139.	-9.8	
1.1	37	1	1	2	-1	.519	.689	41.703	672.	620.	-52.5	
5.0	38	2	1	2	-1	.519	.685	41.810	334.	308.	-25.7	
2.5	39	1	1	2	1	.528	.591	44.213	26.	25.	-.7	
.2	40	2	1	2	1	.528	.587	44.327	13.	12.	-.4	
.1	41	1	1	1	2	.531	.557	45.205	746.	673.	-72.7	
5.7	42	2	1	1	2	.531	.553	45.323	371.	333.	-37.7	
2.8	43	1	2	0	-2	.531	.552	45.360	193.	173.	-19.5	
1.5	44	2	2	0	-2	.531	.548	45.478	96.	87.	-9.1	
.7	45	1	2	1	1	.532	.544	45.611	99.	91.	-8.2	
.8	46	2	2	1	1	.532	.540	45.730	49.	46.	-3.5	
.4	47	1	2	1	-2	.536	.452	48.864	153.	157.	4.1	
1.1	48	2	2	1	-2	.536	.449	48.992	76.	79.	2.7	
.6	49	1	0	2	-2	.536	.431	49.790	433.	482.	49.0	
3.7	50	1	0	2	2	.536	.432	49.774	433.	479.	45.9	
3.7	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
1.9	51	2	0	2	-2	.535	.429	49.921	215.	257.	41.4	
1.9	52	2	0	2	2	.535	.429	49.905	215.	254.	38.9	
13.2	53	1	2	2	0	.535	.421	50.281	1296.	1896.	600.6	
6.6	54	2	2	2	0	.535	.419	50.413	644.	955.	311.4	
7.2	55	1	1	2	-2	.535	.408	50.945	780.	944.	164.5	
3.4	56	2	1	2	-2	.535	.406	51.080	387.	439.	51.2	
4.4	57	1	2	2	-1	.534	.402	51.310	524.	540.	16.5	
2.2	58	2	2	2	-1	.534	.399	51.446	260.	260.	-.2	
.9	59	1	3	0	0	.529	.366	53.804	102.	100.	-2.0	
.4	60	2	3	0	0	.529	.364	53.947	51.	49.	-1.8	

5.3	61	1	2	0	2	.527	.360	54.351	626.	578.	-48.7
2.6	62	2	2	0	2	.527	.359	54.495	311.	287.	-24.3
.3	63	1	1	2	2	.524	.353	55.224	28.	27.	-1.0
.1	64	2	1	2	2	.523	.352	55.372	14.	13.	-.6
1.9	65	1	2	2	1	.523	.350	55.577	222.	205.	-16.4
.9	66	2	2	2	1	.522	.349	55.725	110.	99.	-11.3
2.2	67	1	0	1	-3	.521	.348	55.891	279.	246.	-33.9
2.2	68	1	0	1	3	.521	.349	55.880	280.	246.	-33.7
3.1	69	1	1	1	-3	.521	.348	55.929	393.	344.	-48.2
1.1	70	2	0	1	-3	.521	.348	56.040	139.	122.	-17.1
1.1	71	2	0	1	3	.521	.348	56.029	139.	122.	-17.1
1.6	72	2	1	1	-3	.520	.347	56.079	195.	171.	-23.9
.0	73	1	0	3	-1	.519	.346	56.405	0.	0.	.0
.0	74	1	0	3	1	.519	.346	56.395	0.	0.	.0
3.4	75	1	1	3	0	.518	.345	56.514	406.	358.	-48.5
.0	76	2	0	3	-1	.518	.345	56.557	0.	0.	.0
.0	77	2	0	3	1	.518	.345	56.546	0.	0.	.0
1.7	78	2	1	3	0	.517	.345	56.666	202.	178.	-24.1
3.9	79	1	3	1	-1	.517	.344	56.846	475.	425.	-50.3
.0	80	1	3	1	0	.516	.344	56.920	5.	4.	-.5
2.0	81	2	3	1	-1	.516	.344	56.999	236.	217.	-19.2
.0	82	2	3	1	0	.515	.343	57.073	2.	2.	-.2
.2	83	1	2	1	2	.513	.343	57.443	22.	22.	-.4
.1	84	2	2	1	2	.512	.342	57.598	11.	11.	-.2
1.8	85	1	2	2	-2	.507	.342	58.430	217.	222.	5.0
1.8	86	1	1	3	-1	.507	.342	58.479	220.	227.	6.7
.9	87	2	2	2	-2	.506	.342	58.587	108.	114.	5.8
1.0	88	2	1	3	-1	.506	.342	58.637	109.	116.	7.1
4.5	89	1	3	0	-2	.498	.345	59.660	457.	532.	75.3
2.3	90	2	3	0	-2	.497	.346	59.822	227.	269.	41.7
5.4	91	1	1	3	1	.491	.349	60.461	532.	641.	109.2
2.6	92	2	1	3	1	.490	.350	60.625	264.	301.	37.1
1.7	93	1	1	1	3	.477	.361	61.933	201.	195.	-5.8



2.2	94	1	2	1	-3	.476	.362	62.052	260.	247.	-12.5
.9	95	2	1	1	3	.476	.362	62.102	100.	95.	-5.1
1.2	96	2	2	1	-3	.474	.364	62.222	129.	123.	-6.1
.0	97	1	3	1	-2	.470	.368	62.591	0.	0.	.0
.0	98	2	3	1	-2	.468	.370	62.763	0.	0.	.0
5.2	99	1	3	1	1	.468	.370	62.801	544.	552.	8.0
2.6	100	2	3	1	1	.466	.372	62.973	270.	275.	4.9
	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF
.3	101	1	0	2	-3	.443	.399	64.759	30.	29.	-1.0
.3	102	1	0	2	3	.443	.398	64.738	30.	29.	-1.0
.9	103	1	1	2	-3	.442	.399	64.794	92.	89.	-2.7
.1	104	2	0	2	-3	.440	.402	64.937	15.	14.	-.3
.1	105	2	0	2	3	.440	.402	64.917	15.	14.	-.3
.4	106	2	1	2	-3	.440	.402	64.973	46.	45.	-.7
.2	107	1	0	3	-2	.438	.404	65.054	17.	17.	-.2
.2	108	1	0	3	2	.439	.404	65.034	17.	17.	-.2
.1	109	2	0	3	-2	.436	.407	65.234	9.	8.	.0
.1	110	2	0	3	2	.436	.407	65.213	9.	8.	.0
.3	111	1	2	3	0	.432	.411	65.464	34.	34.	-.1
.1	112	1	3	2	-1	.430	.415	65.631	6.	6.	.0
.2	113	2	2	3	0	.429	.415	65.645	17.	17.	-.1
.6	114	1	3	2	0	.429	.416	65.697	69.	68.	-.5
.0	115	2	3	2	-1	.427	.418	65.812	3.	3.	.0
.3	116	2	3	2	0	.426	.420	65.879	34.	34.	-.4
.8	117	1	1	3	-2	.423	.423	66.031	95.	95.	-.2
1.5	118	1	2	2	2	.421	.426	66.176	178.	186.	8.8
.4	119	2	1	3	-2	.420	.426	66.214	47.	51.	3.4
.3	120	1	2	3	-1	.418	.429	66.339	29.	33.	4.1
.8	121	2	2	2	2	.418	.429	66.359	88.	102.	13.3
.1	122	2	2	3	-1	.415	.433	66.524	14.	17.	2.5
1.0	123	1	1	3	2	.346	.515	69.717	96.	91.	-4.7
.5	124	2	1	3	2	.341	.521	69.914	48.	45.	-2.4
.2	125	1	2	3	1	.338	.525	70.028	18.	17.	-1.0

.1	126	2	2	3	1	.332	.531	70.225	9.	8.	-.6	
.5	127	1	1	2	3	.329	.535	70.346	50.	46.	-3.5	
.5	128	1	2	2	-3	.325	.538	70.468	44.	41.	-3.0	
.3	129	2	1	2	3	.323	.541	70.545	25.	23.	-1.5	
.2	130	2	2	2	-3	.319	.545	70.667	22.	21.	-1.1	
.7	131	1	3	2	-2	.310	.555	70.972	64.	61.	-2.5	
.1	132	1	3	0	2	.309	.556	71.010	8.	8.	-.3	
.1	133	1	3	2	1	.304	.561	71.164	11.	10.	-.3	
.1	134	2	3	2	-2	.303	.561	71.173	32.	31.	-1.0	
.4	135	2	3	0	2	.302	.563	71.212	4.	4.	-.1	
.0	136	2	3	2	1	.297	.568	71.366	5.	5.	-.2	
.1	137	1	1	0	-4	.284	.581	71.743	159.	149.	-10.4	
1.8	138	2	1	0	-4	.276	.588	71.947	79.	75.	-4.3	
.9	139	1	2	3	-2	.251	.611	72.559	51.	49.	-1.4	
.6	140	1	0	0	4	.249	.613	72.611	19.	19.	-.6	
.2	141	2	2	3	-2	.242	.618	72.766	25.	24.	-1.0	
.3	142	2	0	0	4	.239	.620	72.818	10.	9.	-.4	
.1	143	1	2	1	3	.221	.635	73.196	26.	26.	.0	
.3	144	1	3	1	-3	.212	.642	73.373	11.	11.	.0	
.1	145	2	2	1	3	.210	.643	73.405	13.	13.	.1	
.2	146	1	0	4	0	.204	.647	73.505	24.	24.	.5	
.3	147	2	3	1	-3	.200	.650	73.583	6.	6.	.2	
.1	148	1	3	1	2	.193	.655	73.697	0.	0.	.0	
.0	149	2	0	4	0	.192	.655	73.716	12.	13.	1.1	
.2	150	2	3	1	2	.180	.663	73.909	0.	0.	.0	
.0	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
.9	151	1	4	0	0	.158	.676	74.212	58.	60.	1.8	
.4	152	2	4	0	0	.141	.685	74.425	29.	28.	-.5	
.1	153	1	1	1	-4	.140	.685	74.430	4.	4.	-.1	
.0	154	2	1	1	-4	.120	.694	74.644	2.	2.	.0	
.0	155	1	0	1	-4	.010	.722	75.286	0.	0.	.0	
.0	156	1	0	1	4	.010	.721	75.273	0.	0.	.0	
.0	157	2	0	1	-4	.010	.731	75.503	0.	0.	.0	

.0	158	2		0	1	4	.010	.731	75.491	0.	0.	.0
2.5	159	1		4	1	-1	.010	.750	75.912	70.	61.	-9.2
3.4	160	1		0	4	-1	.010	.759	76.113	100.	76.	-23.2
2.6	161	1		0	4	1	.010	.759	76.101	100.	86.	-13.6
.9	162	2		4	1	-1	.010	.760	76.132	35.	30.	-5.1
.7	163	1		1	4	0	.010	.763	76.204	23.	22.	-.8
.0	164	1		2	0	-4	.010	.768	76.308	0.	0.	.0
1.3	165	2		0	4	-1	.010	.769	76.334	50.	45.	-4.7
2.0	166	2		0	4	1	.010	.769	76.321	50.	43.	-6.3
.4	167	2		1	4	0	.010	.774	76.426	12.	11.	-.4
.0	168	2		2	0	-4	.010	.779	76.530	0.	0.	.0
1.4	169	1		4	1	0	.010	.794	76.859	51.	47.	-4.2
1.0	170	2		4	1	0	.010	.805	77.083	25.	24.	-1.6
.8	171	1		4	0	-2	.010	.825	77.490	29.	26.	-2.4
.4	172	2		4	0	-2	.010	.837	77.716	14.	14.	.1
.1	173	1		1	4	-1	.010	.846	77.906	2.	2.	-.1
.0	174	2		1	4	-1	.010	.858	78.134	1.	1.	-.1
.1	175	1		0	3	-3	.010	.867	78.312	3.	3.	-.1
.1	176	1		0	3	3	.010	.866	78.284	3.	3.	-.1
.1	177	1		1	3	-3	.010	.869	78.344	3.	3.	-.1
.0	178	2		0	3	-3	.010	.879	78.542	2.	2.	.0
.0	179	2		0	3	3	.010	.878	78.514	2.	2.	.0
.0	180	2		1	3	-3	.010	.881	78.574	2.	2.	.0
.4	181	1		1	0	4	.010	.895	78.846	14.	12.	-1.4
1.0	182	1		2	1	-4	.010	.900	78.939	36.	33.	-2.6
.2	183	2		1	0	4	.010	.908	79.078	7.	6.	-.6
.6	184	1		3	3	-1	.010	.910	79.115	16.	14.	-1.9
.5	185	2		2	1	-4	.010	.913	79.172	18.	17.	-1.1
1.2	186	1		3	3	0	.010	.913	79.175	37.	35.	-2.0
.4	187	2		3	3	-1	.010	.923	79.348	8.	8.	-.1
.7	188	2		3	3	0	.010	.926	79.409	18.	18.	-.6
.4	189	1		2	3	2	.010	.937	79.617	10.	9.	-1.1
.3	190	1		1	4	1	.010	.939	79.644	7.	6.	-.3

.2	191	2	2	3	2	.010	.951	79.852	5.	5.	-.1	
.1	192	2	1	4	1	.010	.952	79.879	3.	3.	-.2	
.4	193	1	4	1	-2	.010	.965	80.106	11.	10.	-.4	
.2	194	2	4	1	-2	.010	.978	80.343	5.	5.	-.2	
.2	195	1	2	2	3	.010	1.022	81.088	6.	6.	-.1	
.3	196	1	3	2	-3	.010	1.032	81.268	7.	7.	-.4	
.1	197	2	2	2	3	.010	1.036	81.329	3.	3.	-.1	
.1	198	1	1	1	4	.010	1.043	81.442	4.	4.	.3	
.1	199	2	3	2	-3	.010	1.047	81.510	4.	4.	.2	
.0	200	1	3	2	2	.010	1.051	81.575	0.	0.	.0	
	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
.1	201	2	1	1	4	.010	1.057	81.685	2.	2.	.2	
.0	202	2	3	2	2	.010	1.066	81.818	0.	0.	.0	
2.1	203	1	1	2	-4	.010	1.095	82.296	54.	56.	1.5	
1.0	204	2	1	2	-4	.010	1.110	82.542	27.	31.	3.7	
.2	205	1	4	1	1	.010	1.133	82.898	8.	8.	-.2	
.3	206	1	0	2	-4	.010	1.148	83.129	11.	10.	-.3	
.4	207	1	0	2	4	.010	1.146	83.105	11.	10.	-.5	
.2	208	2	4	1	1	.010	1.149	83.147	4.	4.	.0	
.2	209	2	0	2	-4	.010	1.164	83.379	5.	5.	-.3	
.2	210	2	0	2	4	.010	1.162	83.355	5.	5.	-.4	
2.4	211	1	1	3	3	.010	1.174	83.532	80.	76.	-4.4	
2.5	212	1	2	3	-3	.010	1.182	83.656	90.	90.	.8	
.2	213	1	4	2	-1	.010	1.187	83.734	5.	5.	-.1	
.2	214	1	0	4	-2	.010	1.190	83.775	4.	3.	-.4	
.1	215	1	0	4	2	.010	1.188	83.750	4.	4.	-.1	
1.2	216	2	1	3	3	.010	1.191	83.784	40.	37.	-3.2	
1.7	217	2	2	3	-3	.010	1.199	83.908	45.	42.	-2.2	
.1	218	2	4	2	-1	.010	1.204	83.987	3.	3.	.0	
.1	219	2	0	4	-2	.010	1.207	84.028	2.	2.	.1	
.1	220	2	0	4	2	.010	1.205	84.003	2.	2.	.0	
.9	221	1	3	3	-2	.010	1.214	84.133	24.	22.	-2.3	
.9	222	1	2	4	0	.010	1.215	84.146	29.	26.	-2.2	

223	1	3	3	1	.010	1.226	84.311	19.	19.	-.4		
.7	224	2	3	3	-2	.010	1.231	84.387	12.	11.	-1.0	
.3	225	2	2	4	0	.010	1.232	84.401	14.	12.	-1.8	
.6	226	2	3	3	1	.010	1.243	84.566	10.	9.	-.5	
.4	227	1	4	2	0	.010	1.249	84.658	56.	50.	-5.5	
1.9	228	1	1	4	-2	.010	1.250	84.668	12.	11.	-1.4	
.5	229	2	4	2	0	.010	1.267	84.915	28.	26.	-1.9	
.8	230	2	1	4	-2	.010	1.268	84.926	6.	6.	-.6	
.2	231	1	2	4	-1	.010	1.269	84.950	26.	25.	-1.2	
.8	232	2	2	4	-1	.010	1.287	85.208	13.	14.	1.0	
.4	233	1	3	0	-4	.010	1.346	86.036	60.	56.	-3.5	
1.7	234	2	3	0	-4	.010	1.365	86.299	30.	30.	-.1	
.9	235	1	2	2	-4	.010	1.395	86.704	10.	10.	-.5	
.4	236	2	2	2	-4	.010	1.414	86.971	5.	5.	-.3	
.2	237	1	4	2	-2	.010	1.481	87.849	7.	7.	-.1	
.2	238	1	1	4	2	.010	1.499	88.084	7.	7.	-.3	
.2	239	2	4	2	-2	.010	1.502	88.121	3.	3.	-.1	
.1	240	2	1	4	2	.010	1.520	88.357	4.	3.	-.2	
.1	241	1	2	4	1	.010	1.522	88.377	62.	60.	-2.1	
1.7	242	1	3	1	-4	.010	1.540	88.608	7.	7.	-.1	
.2	243	2	2	4	1	.010	1.543	88.651	31.	29.	-1.8	
1.1	244	2	3	1	-4	.010	1.561	88.883	4.	3.	-.2	
.1	245	1	3	1	3	.010	1.574	89.043	80.	74.	-6.0	
2.5	246	1	1	2	4	.010	1.583	89.160	69.	60.	-9.3	
2.2	247	1	4	1	-3	.010	1.593	89.278	81.	70.	-11.1	
2.5	248	2	3	1	3	.010	1.596	89.321	40.	33.	-6.4	
1.3	249	2	1	2	4	.010	1.606	89.438	34.	32.	-2.8	
1.0	250	2	4	1	-3	.010	1.615	89.556	40.	34.	-5.8	
1.2	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
1.4	251	1	2	0	4	.010	1.665	90.169	43.	39.	-4.7	
.6	252	2	2	0	4	.010	1.689	90.452	22.	19.	-2.2	
1.2	253	1	4	2	1	.010	1.702	90.606	33.	30.	-3.8	
1.0	254	1	2	4	-2	.010	1.716	90.779	30.	29.	-1.1	

.5	255	2	4	2	1	.010	1.726	90.891	17.	15.	-1.6
.6	256	2	2	4	-2	.010	1.740	91.065	15.	13.	-2.1
.7	257	1	4	0	2	.010	1.762	91.319	21.	21.	-.5
.3	258	2	4	0	2	.010	1.787	91.608	11.	10.	-.3
.2	259	1	2	1	4	.010	1.885	92.727	6.	6.	.1
.1	260	2	2	1	4	.010	1.912	93.023	3.	3.	-.2
.0	261	1	4	1	2	.010	1.990	93.882	0.	0.	.0
.5	262	1	2	3	3	.010	1.995	93.942	17.	16.	-.1
.2	263	1	3	3	-3	.010	2.013	94.130	7.	7.	.4
.0	264	2	4	1	2	.010	2.018	94.184	0.	0.	.0
.3	265	2	2	3	3	.010	2.024	94.245	8.	9.	.7
.1	266	2	3	3	-3	.010	2.041	94.434	3.	3.	-.2
1.4	267	1	3	3	2	.010	2.040	94.427	46.	44.	-2.2
.8	268	2	3	3	2	.010	2.069	94.732	23.	26.	2.6
.1	269	1	1	3	-4	.010	2.109	95.153	3.	3.	.3
.1	270	2	1	3	-4	.010	2.139	95.462	2.	2.	.2
.5	271	1	0	3	-4	.010	2.189	95.984	14.	15.	.4
.5	272	1	0	3	4	.010	2.186	95.947	14.	16.	1.9
.2	273	2	0	3	-4	.010	2.220	96.297	7.	7.	-.4
.2	274	2	0	3	4	.010	2.216	96.260	7.	7.	.1
1.5	275	1	3	2	-4	.010	2.222	96.319	52.	49.	-3.5
.3	276	1	0	4	-3	.010	2.226	96.360	11.	10.	-.8
.3	277	1	0	4	3	.010	2.223	96.323	11.	10.	-.7
.1	278	1	1	1	-5	.010	2.228	96.374	3.	2.	-.2
.7	279	1	1	4	-3	.010	2.229	96.391	26.	24.	-2.1
1.4	280	1	4	3	-1	.010	2.248	96.583	46.	46.	-.1
.8	281	2	3	2	-4	.010	2.253	96.634	26.	24.	-1.9
.2	282	2	0	4	-3	.010	2.257	96.676	5.	5.	-.1
.1	283	2	0	4	3	.010	2.254	96.639	5.	5.	-.3
.0	284	2	1	1	-5	.010	2.259	96.690	1.	1.	.0
.4	285	2	1	4	-3	.010	2.261	96.707	13.	13.	-.3
.0	286	1	3	2	3	.010	2.264	96.746	1.	1.	.0
.7	287	2	4	3	-1	.010	2.280	96.899	23.	23.	-.3

288	1	4	2	-3	.010	2.289	96.991	3.	3.	-.1	
.1	289	2	3	2	3	.010	2.296	97.064	0.	0.	.0
.0	290	1	3	4	-1	.010	2.305	97.149	39.	37.	-1.1
1.2	291	1	3	4	0	.010	2.311	97.207	1.	1.	.0
.0	292	2	4	2	-3	.010	2.321	97.310	1.	1.	-.1
.0	293	2	3	4	-1	.010	2.337	97.469	19.	18.	-.9
.6	294	1	4	3	0	.010	2.341	97.507	7.	6.	-.7
.2	295	2	3	4	0	.010	2.343	97.528	1.	1.	-.1
.0	296	1	2	4	2	.010	2.355	97.642	15.	15.	-.3
.5	297	2	4	3	0	.010	2.374	97.829	3.	3.	-.2
.1	298	1	5	0	0	.010	2.381	97.896	24.	22.	-2.0
.7	299	2	2	4	2	.010	2.388	97.965	8.	7.	-.4
.2	300	1	0	1	-5	.010	2.399	98.072	30.	27.	-2.1
.9											

	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
.7	301	1	0	1	5	.010	2.397	98.057	30.	27.	-2.2	
.3	302	2	5	0	0	.010	2.414	98.220	12.	11.	-.5	
.4	303	2	0	1	-5	.010	2.432	98.397	15.	15.	-.2	
.5	304	2	0	1	5	.010	2.431	98.382	15.	15.	-.1	
.2	305	1	5	1	-1	.010	2.463	98.688	6.	5.	-.4	
.1	306	2	5	1	-1	.010	2.497	99.017	3.	3.	-.1	
.0	307	1	0	5	-1	.010	2.534	99.370	0.	0.	.0	
.0	308	1	0	5	1	.010	2.533	99.354	0.	0.	.0	
.6	309	1	5	0	-2	.010	2.535	99.374	20.	20.	-.6	
1.1	310	1	1	5	0	.010	2.544	99.458	37.	34.	-3.0	
.8	311	1	2	3	-4	.010	2.557	99.577	31.	30.	-.5	
.0	312	2	0	5	-1	.010	2.570	99.703	0.	0.	.0	
.0	313	2	0	5	1	.010	2.568	99.687	0.	0.	.0	
.2	314	2	5	0	-2	.010	2.570	99.707	10.	10.	-.1	
.6	315	2	1	5	0	.010	2.579	99.791	19.	19.	.0	
.4	316	2	2	3	-4	.010	2.592	99.911	15.	15.	.0	
1.1	317	1	2	1	-5	.010	2.595	99.940	40.	40.	-.1	

DERIVED BRAGG R-FACTOR=						12.						
	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
11.4	1	1	1	1	0	.285	.348	32.531	993.	1077.	84.0	

5.7	2	2	1	1	0	.285	.352	32.614	494.	533.	39.6
24.5	3	1	0	0	2	.263	.490	35.453	3742.	3735.	-7.4
10.9	4	2	0	0	2	.262	.494	35.543	1861.	1890.	29.8
60.9	5	1	1	1	-1	.262	.496	35.572	10382.	10598.	215.5
33.0	6	2	1	1	-1	.261	.500	35.662	5162.	5282.	119.3
76.2	7	1	1	1	1	.244	.618	38.730	13412.	13050.	-362.6
37.7	8	2	1	1	1	.244	.621	38.829	6668.	6517.	-150.9
19.9	9	1	2	0	0	.243	.626	38.976	2841.	2789.	-52.3
11.4	10	2	2	0	0	.243	.629	39.076	1413.	1367.	-45.4
3.0	11	1	1	1	-2	.242	.780	46.292	270.	260.	-9.9
1.5	12	2	1	1	-2	.242	.781	46.413	134.	131.	-3.3
31.9	13	1	2	0	-2	.255	.794	48.826	3748.	3817.	68.5
15.9	14	2	2	0	-2	.256	.794	48.954	1863.	1902.	38.9
1.7	15	1	1	1	2	.274	.787	51.361	175.	176.	.9
.9	16	2	1	1	2	.275	.786	51.497	87.	85.	-1.9
12.7	17	1	0	2	0	.295	.764	53.509	1340.	1323.	-16.6
6.5	18	2	0	2	0	.296	.762	53.651	666.	664.	-1.5
.5	19	1	0	2	-1	.333	.703	56.739	55.	48.	-6.6
.5	20	1	0	2	1	.333	.703	56.754	54.	48.	-6.5
.2	21	2	0	2	-1	.335	.699	56.891	27.	24.	-2.8
.2	22	2	0	2	1	.335	.699	56.906	27.	24.	-2.7
16.4	23	1	2	0	2	.353	.662	58.287	1899.	1921.	22.0
8.1	24	2	2	0	2	.355	.657	58.444	944.	958.	14.4
21.5	25	1	1	1	-3	.401	.549	61.584	2499.	2626.	127.4
10.5	26	2	1	1	-3	.403	.542	61.752	1242.	1266.	24.1
8.0	27	1	0	2	-2	.470	.351	65.825	967.	957.	-10.2
8.0	28	1	0	2	2	.470	.350	65.854	966.	956.	-10.4
3.9	29	2	0	2	-2	.473	.342	66.008	481.	481.	.0
3.9	30	2	0	2	2	.473	.340	66.036	480.	483.	2.7
16.4	31	1	3	1	-1	.478	.324	66.327	1855.	2096.	240.8
8.7	32	2	3	1	-1	.481	.314	66.511	922.	1075.	153.3
.5	33	1	3	1	0	.482	.312	66.543	55.	64.	9.0
.3	34	2	3	1	0	.485	.302	66.728	27.	30.	3.0



9.4	35	1	1	1	3	.506	.233	67.913	1094.	1113.	18.3	
4.6	36	2	1	1	3	.510	.222	68.103	544.	554.	10.3	
14.1	37	1	2	2	0	.510	.220	68.137	1682.	1710.	27.3	
7.1	38	2	2	2	0	.514	.208	68.328	836.	826.	-10.5	
.4	39	1	2	2	-1	.525	.170	68.941	45.	44.	-1.4	
.2	40	2	2	2	-1	.528	.158	69.135	23.	22.	-.6	
.4	41	1	3	1	-2	.579	-.024	71.803	39.	37.	-2.4	
.2	42	2	3	1	-2	.583	-.039	72.007	20.	18.	-1.1	
7.8	43	1	3	1	1	.591	-.070	72.428	850.	819.	-31.4	
3.9	44	2	3	1	1	.595	-.086	72.635	423.	408.	-14.5	
.3	45	1	2	2	1	.602	-.112	72.977	35.	34.	-.8	
.2	46	2	2	2	1	.606	-.128	73.186	17.	17.	-.1	
6.5	47	1	0	0	4	.643	-.275	75.026	683.	718.	35.0	
3.2	48	2	0	0	4	.648	-.293	75.242	340.	351.	11.0	
6.7	49	1	2	2	-2	.649	-.298	75.312	721.	736.	15.4	
3.3	50	2	2	2	-2	.654	-.317	75.530	358.	351.	-7.5	
	NO.	CODE	H	K	L	HW	SHAPE	POSN	ICALC	COBS	DIFF	ESD
.1	51	1	0	2	-3	.745	-.702	79.754	12.	12.	-.4	
.1	52	1	0	2	3	.746	-.706	79.793	12.	12.	-.4	
.1	53	2	0	2	-3	.751	-.725	79.990	6.	6.	-.2	
.1	54	2	0	2	3	.751	-.729	80.029	6.	6.	-.2	
2.2	55	1	2	0	-4	.758	-.756	80.301	222.	212.	-10.0	
.2	56	1	1	1	-4	.758	-.758	80.326	24.	23.	-1.1	
1.1	57	2	2	0	-4	.763	-.780	80.539	110.	105.	-5.7	
.1	58	2	1	1	-4	.764	-.782	80.564	12.	11.	-.6	
5.5	59	1	3	1	-3	.809	-.984	82.511	520.	569.	49.2	
2.6	60	2	3	1	-3	.815	-1.011	82.758	259.	272.	13.5	
5.0	61	1	2	2	2	.822	-1.046	83.084	501.	500.	-1.1	
2.5	62	2	2	2	2	.828	-1.073	83.334	249.	244.	-5.3	
.2	63	1	3	1	2	.832	-1.092	83.510	21.	20.	-.5	
4.5	64	1	4	0	0	.837	-1.114	83.705	450.	442.	-8.7	
.1	65	2	3	1	2	.839	-1.120	83.762	10.	10.	-.2	
2.3	66	2	4	0	0	.843	-1.142	83.958	224.	221.	-3.5	

1.8	67	1	4	0	-2	.912	-1.464	86.737	170.	165.	-5.2
.2	68	1	2	2	-3	.915	-1.477	86.842	17.	17.	-.6
.9	69	2	4	0	-2	.919	-1.496	87.003	85.	82.	-2.8
.1	70	2	2	2	-3	.922	-1.509	87.110	9.	8.	-.3
.2	71	1	1	1	4	.945	-1.618	87.999	17.	17.	.1
.0	72	1	1	3	0	.948	-1.635	88.130	0.	0.	.0
.1	73	2	1	1	4	.952	-1.652	88.272	9.	9.	.0
.0	74	2	1	3	0	.955	-1.669	88.403	0.	0.	.0
7.3	75	1	1	3	-1	.993	-1.851	89.826	709.	639.	-69.9
3.7	76	2	1	3	-1	1.001	-1.888	90.107	354.	322.	-31.1
3.1	77	1	1	3	1	1.046	-2.107	91.746	284.	270.	-14.9
1.6	78	2	1	3	1	1.054	-2.147	92.037	142.	132.	-10.0
1.5	79	1	2	0	4	1.157	-2.651	95.560	127.	142.	15.6
.7	80	2	2	0	4	1.167	-2.697	95.871	63.	68.	4.8
.0	81	1	1	3	-2	1.197	-2.845	96.849	0.	0.	.0
.0	82	2	1	3	-2	1.207	-2.894	97.168	0.	0.	.0
.1	83	1	2	2	3	1.243	-3.072	98.315	12.	11.	-.7
.1	84	1	3	1	-4	1.242	-3.069	98.297	12.	12.	-.8
1.4	85	1	0	2	-4	1.246	-3.089	98.422	149.	140.	-9.3
1.3	86	1	0	2	4	1.248	-3.097	98.474	149.	140.	-9.4
.1	87	2	2	2	3	1.253	-3.124	98.642	6.	6.	-.4
.1	88	2	3	1	-4	1.253	-3.121	98.624	6.	6.	-.4
.6	89	2	0	2	-4	1.257	-3.141	98.750	75.	70.	-4.8
.6	90	2	0	2	4	1.259	-3.149	98.802	75.	70.	-4.8
5.2	91	1	3	1	3	1.288	-3.294	99.703	443.	426.	-17.0

DERIVED BRAGG R-FACTOR= 2.9