

```
start_X 3.5
finish_X 39.0
Zero_Error( 0.03)
LP_Factor( 90)
convolution_step 2
Rp 100
Rs 100
lam
ymin_on_ymax 0.0001
la 1 lo 1.238879 lh 1e-006
```

```

x_calculation_step 0.02
}

macro RB_1 {

site Cu41 x 0.00000_0.00000 y 0.00000_0.00000 z 0.00000_0.00000 occ Cu 1 beq !b1 7.1342_0.1385
site N4 x -0.06474_0.00000 y 0.13717_0.00000 z -0.07588_0.00000 occ N 1 beq !b1 7.1342_0.1385
site N10 x 0.26430_0.00000 y 0.06503_0.00000 z 0.13135_0.00000 occ N 1 beq !b1 7.1342_0.1385
site C2 x -0.23631_0.00000 y 0.15580_0.00000 z -0.17851_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C5 x 0.05546_0.00000 y 0.22748_0.00000 z -0.03348_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C11 x 0.40504_0.00000 y 0.01520_0.00000 z 0.22541_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C12 x 0.33375_0.00000 y 0.16649_0.00000 z 0.14179_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C1 x -0.22631_0.00000 y 0.26100_0.00000 z -0.20286_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C3 x -0.04156_0.00000 y 0.30672_0.00000 z -0.11113_0.00000 occ C 1 beq !b1 7.1342_0.1385
site N39 x 0.23903_0.00000 y 0.24193_0.00000 z 0.06653_0.00000 occ N 1 beq !b1 7.1342_0.1385
site C13 x 0.56956_0.00000 y 0.08643_0.00000 z 0.29839_0.00000 occ C 1 beq !b1 7.1342_0.1385
site N38 x 0.39374_0.00000 y -0.08631_0.00000 z 0.24797_0.00000 occ N 1 beq !b1 7.1342_0.1385
site C14 x 0.52440_0.00000 y 0.18240_0.00000 z 0.24538_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C6 x -0.36275_0.00000 y 0.32036_0.00000 z -0.29720_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C8 x 0.01638_0.00000 y 0.41383_0.00000 z -0.10883_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C15 x 0.75377_0.00000 y 0.07532_0.00000 z 0.40604_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C17 x 0.66140_0.00000 y 0.27214_0.00000 z 0.29747_0.00000 occ C 1 beq !b1 7.1342_0.1385
site C7 x -0.30683_0.00000 y 0.42784_0.00000 z -0.29616_0.00000 occ C 1 beq !b1 7.1342_0.1385
site H42 x -0.49908_0.00000 y 0.28674_0.00000 z -0.36493_0.00000 occ H 1 beq !b1 7.1342_0.1385
site C9 x -0.11876_0.00000 y 0.47436_0.00000 z -0.20276_0.00000 occ C 1 beq !b1 7.1342_0.1385
site H44 x 0.15280_0.00000 y 0.44718_0.00000 z -0.04098_0.00000 occ H 1 beq !b1 7.1342_0.1385
site C16 x 0.89256_0.00000 y 0.16455_0.00000 z 0.45930_0.00000 occ C 1 beq !b1 7.1342_0.1385
site H46 x 0.78678_0.00000 y 0.00452_0.00000 z 0.44498_0.00000 occ H 1 beq !b1 7.1342_0.1385
site C18 x 0.84672_0.00000 y 0.26227_0.00000 z 0.40541_0.00000 occ C 1 beq !b1 7.1342_0.1385
site H48 x 0.62820_0.00000 y 0.34288_0.00000 z 0.25845_0.00000 occ H 1 beq !b1 7.1342_0.1385
site H43 x -0.40352_0.00000 y 0.47254_0.00000 z -0.36376_0.00000 occ H 1 beq !b1 7.1342_0.1385
site H45 x -0.07997_0.00000 y 0.55237_0.00000 z -0.20303_0.00000 occ H 1 beq !b1 7.1342_0.1385
site H47 x 1.02736_0.00000 y 0.15840_0.00000 z 0.53752_0.00000 occ H 1 beq !b1 7.1342_0.1385
site H49 x 0.94866_0.00000 y 0.32638_0.00000 z 0.44493_0.00000 occ H 1 beq !b1 7.1342_0.1385

rigid
z_matrix Cu41
z_matrix N4 Cu41 =1.9983;
z_matrix N10 Cu41 =1.9968; N4 90.162
z_matrix C2 N4 =1.3600; Cu41 125.894 N10 -180
z_matrix C5 N4 =1.3559; Cu41 125.622 C2 180
z_matrix C11 N10 =1.3601; Cu41 125.851 N4 -180
z_matrix C12 N10 =1.3560; Cu41 125.694 C11 180
z_matrix C1 C2 =1.3993; N4 109.123 Cu41 180
z_matrix C3 C5 =1.4061; N4 108.943 Cu41 -180
z_matrix N39 C5 =1.3508; N4 126.948 C3 180
z_matrix C13 C11 =1.3989; N10 109.176 Cu41 180
z_matrix N38 C11 =1.3484; N10 127.018 C13 -180
z_matrix C14 C12 =1.4021; N10 108.925 Cu41 -180

```

z\_matrix C6 C1 =1.4196; C2 132.099 N4 180  
 z\_matrix C8 C3 =1.4154; C5 132.063 N4 180  
 z\_matrix C15 C13 =1.4195; C11 132.067 N10 -180  
 z\_matrix C17 C14 =1.4156; C12 132.123 N10 180  
 z\_matrix C7 C6 =1.4186; C1 118.280 C2 180  
 z\_matrix H42 C6 =1.0302; C1 121.233 C7 180  
 z\_matrix C9 C8 =1.4226; C3 118.274 C5 180  
 z\_matrix H44 C8 =1.0300; C3 120.944 C9 180  
 z\_matrix C16 C15 =1.4183; C13 118.281 C11 180  
 z\_matrix H46 C15 =1.0301; C13 121.268 C16 -180  
 z\_matrix C18 C17 =1.4229; C14 118.305 C12 -180  
 z\_matrix H48 C17 =1.0299; C14 121.016 C18 -180  
 z\_matrix H43 C7 =1.0313; C6 119.666 C1 180  
 z\_matrix H45 C9 =1.0285; C8 119.691 C3 -180  
 z\_matrix H47 C16 =1.0311; C15 119.686 C13 180  
 z\_matrix H49 C18 =1.0285; C17 119.716 C14 -180

rotate -47.14425\_0.07259 min -67 max -38 qa 1 operate\_on\_points "C\* H\* N\* "  
 rotate -235.43697\_0.05761 min -253 max -223 qb 1 operate\_on\_points "C\* H\* N\* "  
 rotate 42.58863\_0.08530 min 37 max 67 qc 1 operate\_on\_points "C\* H\* N\* "  
 }

macro RB\_2{

site Cu41 x 0.00000\_0.00000 y 0.00000\_0.00000 z 0.00000\_0.00000 occ Cu 1 beq !b1 7.1342\_0.1385  
 site N4 x 0.07263\_0.00000 y -0.21640\_0.00000 z 0.09994\_0.00000 occ N 1 beq !b1 7.1342\_0.1385  
 site N10 x 0.13476\_0.00000 y 0.19599\_0.00000 z 0.03057\_0.00000 occ N 1 beq !b1 7.1342\_0.1385  
 site C2 x 0.02714\_0.00000 y -0.41055\_0.00000 z 0.12279\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C5 x 0.17584\_0.00000 y -0.19408\_0.00000 z 0.15647\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C11 x 0.14824\_0.00000 y 0.39325\_0.00000 z -0.01241\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C12 x 0.22840\_0.00000 y 0.15468\_0.00000 z 0.09781\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C1 x 0.10313\_0.00000 y -0.51614\_0.00000 z 0.19604\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C3 x 0.19752\_0.00000 y -0.37944\_0.00000 z 0.21759\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site N39 x 0.24824\_0.00000 y -0.02417\_0.00000 z 0.15615\_0.00000 occ N 1 beq !b1 7.1342\_0.1385  
 site C13 x 0.25335\_0.00000 y 0.48142\_0.00000 z 0.02820\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site N38 x 0.07436\_0.00000 y 0.49346\_0.00000 z -0.08299\_0.00000 occ N 1 beq !b1 7.1342\_0.1385  
 site C14 x 0.30422\_0.00000 y 0.33015\_0.00000 z 0.09812\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C6 x 0.09770\_0.00000 y -0.71954\_0.00000 z 0.24547\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C8 x 0.29114\_0.00000 y -0.43861\_0.00000 z 0.28945\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C15 x 0.30833\_0.00000 y 0.68009\_0.00000 z 0.00991\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C17 x 0.41274\_0.00000 y 0.37011\_0.00000 z 0.15329\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site C7 x 0.19088\_0.00000 y -0.78115\_0.00000 z 0.31770\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site H42 x 0.02813\_0.00000 y -0.82054\_0.00000 z 0.22964\_0.00000 occ H 1 beq !b1 7.1342\_0.1385  
 site C9 x 0.28695\_0.00000 y -0.64197\_0.00000 z 0.33963\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site H44 x 0.36055\_0.00000 y -0.33722\_0.00000 z 0.30509\_0.00000 occ H 1 beq !b1 7.1342\_0.1385  
 site C16 x 0.41711\_0.00000 y 0.72241\_0.00000 z 0.06462\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site H46 x 0.27071\_0.00000 y 0.79137\_0.00000 z -0.04165\_0.00000 occ H 1 beq !b1 7.1342\_0.1385  
 site C18 x 0.46896\_0.00000 y 0.56854\_0.00000 z 0.13580\_0.00000 occ C 1 beq !b1 7.1342\_0.1385  
 site H48 x 0.45026\_0.00000 y 0.25870\_0.00000 z 0.20481\_0.00000 occ H 1 beq !b1 7.1342\_0.1385

```

site H43 x 0.18884_0.00000 y -0.92819_0.00000 z 0.35457_0.00000 occ H 1 beq lb1 7.1342_0.1385
site H45 x 0.35397_0.00000 y -0.68851_0.00000 z 0.39216_0.00000 occ H 1 beq lb1 7.1342_0.1385
site H47 x 0.45871_0.00000 y 0.86563_0.00000 z 0.05262_0.00000 occ H 1 beq lb1 7.1342_0.1385
site H49 x 0.54787_0.00000 y 0.60119_0.00000 z 0.17498_0.00000 occ H 1 beq lb1 7.1342_0.1385

```

rigid

```

z_matrix Cu41
z_matrix N4 Cu41 =1.9983;
z_matrix N10 Cu41 =1.9968; N4 90.162
z_matrix C2 N4 =1.3600; Cu41 125.894 N10 -180
z_matrix C5 N4 =1.3559; Cu41 125.622 C2 180
z_matrix C11 N10 =1.3601; Cu41 125.851 N4 -180
z_matrix C12 N10 =1.3560; Cu41 125.694 C11 180
z_matrix C1 C2 =1.3993; N4 109.123 Cu41 180
z_matrix C3 C5 =1.4061; N4 108.943 Cu41 -180
z_matrix N39 C5 =1.3508; N4 126.948 C3 180
z_matrix C13 C11 =1.3989; N10 109.176 Cu41 180
z_matrix N38 C11 =1.3484; N10 127.018 C13 -180
z_matrix C14 C12 =1.4021; N10 108.925 Cu41 -180
z_matrix C6 C1 =1.4196; C2 132.099 N4 180
z_matrix C8 C3 =1.4154; C5 132.063 N4 180
z_matrix C15 C13 =1.4195; C11 132.067 N10 -180
z_matrix C17 C14 =1.4156; C12 132.123 N10 180
z_matrix C7 C6 =1.4186; C1 118.280 C2 180
z_matrix H42 C6 =1.0302; C1 121.233 C7 180
z_matrix C9 C8 =1.4226; C3 118.274 C5 180
z_matrix H44 C8 =1.0300; C3 120.944 C9 180
z_matrix C16 C15 =1.4183; C13 118.281 C11 180
z_matrix H46 C15 =1.0301; C13 121.268 C16 -180
z_matrix C18 C17 =1.4229; C14 118.305 C12 -180
z_matrix H48 C17 =1.0299; C14 121.016 C18 -180
z_matrix H43 C7 =1.0313; C6 119.666 C1 180
z_matrix H45 C9 =1.0285; C8 119.691 C3 -180
z_matrix H47 C16 =1.0311; C15 119.686 C13 180
z_matrix H49 C18 =1.0285; C17 119.716 C14 -180

```

```

rotate -222.81660 min -237 max -207 qa 1 operate_on_points "C* H* N* "
rotate -199.01401 min -214 max -184 qb 1 operate_on_points "C* H* N* "
rotate 28.83002 min 13 max 43 qc 1 operate_on_points "C* H* N* "

```

}

xdd a\_CPC\_250C010001.xy

```

bkg @ 2328.79483` -119.550066` 28.4579435` -23.8571704` -30.2567324` 53.910911` -8.77749769`
4.0169548` -19.1821231` -14.9122865` 22.2982359`

```

information

str space\_group P-1

r\_bragg 0.320965867

prm scale\_a1 = -(scale\_b1\*mb\*vb\*(Exp(-((k\*t1)^n)))/(ma\*va\*(Exp(-((k\*t1)^n))-1));:0.00071`  
scale =scale\_a1;; 0.0007129013`

phase\_name a-cpc  
cell\_mass 576.081  
cell\_volume 605.1501

weight\_percent wa1 99.999

Phase\_LAC\_1\_on\_cm( 41.31710)  
Phase\_Density\_g\_on\_cm3( 1.58077)  
CS\_G(, 25.10749\_0.33412)  
Strain\_L(, 2.62461\_0.07480)

Out(wa1, " Anteil\_a1:\t %11.5f", "error:\t%11.5f")

Out(scale\_a1, " Skalierung\_a1:\t %11.5f", "error:\t%11.5f")

a 3.83112\_0.00166  
b 13.03000\_0.00149  
c 12.21495\_0.00210  
al 88.99493\_0.03895  
be 96.95233\_0.05200  
ga 89.48921\_0.06164

RB\_1

str CS\_G(, 132.20025\_4.32425)  
Strain\_L(, 0.36128\_0.00985)  
r\_bragg 0.657910104  
phase\_name b-cpc  
cell\_mass 1152.162  
cell\_volume 1215.3144

weight\_percent wb1 0.001

scale =scale\_b1;;0.0000000011`

Out(wb1, " Anteil\_b1:\t %11.5f", "error:\t%11.5f")

Out(scale\_b1, " Skalierung\_b1:\t %11.5f", "error:\t%11.5f")

space\_group P21/c  
Phase\_LAC\_1\_on\_cm( 41.14663)  
Phase\_Density\_g\_on\_cm3( 1.57425)  
a 14.78794\_0.00076

b 4.82142\_0.00020  
c 19.87957\_0.00071  
  
be 120.97069\_0.00481

## RB\_2

xdd a\_CPC\_250C010002.xy

bkg @ 2331.80947` -115.341774` 26.800582` -23.2326414` -28.7402642` 51.658398` -6.91947326`  
2.13750383` -17.9250792` -14.6691222` 21.7817105`

## information

str space\_group P-1  
r\_bragg 0.309688686

prm scale\_a2 = -(scale\_b2\*mb\*vb\*(Exp(-((k\*t2)^n))))/(ma\*va\*((Exp(-((k\*t2)^n))-1));:0.00072`  
scale =scale\_a2;: 0.0007189184`

phase\_name a-cpc  
cell\_mass 576.081  
cell\_volume 605.1501

weight\_percent wa2 99.997

Phase\_LAC\_1\_on\_cm( 41.31710)  
Phase\_Density\_g\_on\_cm3( 1.58077)  
CS\_G(, 25.10749\_0.33412)  
Strain\_L(, 2.62461\_0.07480)

Out(wa2, " Anteil\_a2:\t %11.5f", "error:\t%11.5f")

Out(scale\_a2, " Skalierung\_a2:\t %11.5f", "error:\t%11.5f")

a 3.83112\_0.00166  
b 13.03000\_0.00149  
c 12.21495\_0.00210  
al 88.99493\_0.03895  
be 96.95233\_0.05200  
ga 89.48921\_0.06164

## RB\_1

str CS\_G(, 132.20025\_4.32425)  
Strain\_L(, 0.36128\_0.00985)  
r\_bragg 0.702041326  
phase\_name b-cpc  
cell\_mass 1152.162

cell\_volume 1215.3144

weight\_percent wb2 0.003

scale =scale\_b2;:0.0000000061`

Out(wb2, " Anteil\_b2:\ %11.5f", "error:\t%11.5f")

Out(scale\_b2, " Skalierung\_b2:\ %11.5f", "error:\t%11.5f\n")

space\_group P21/c

Phase\_LAC\_1\_on\_cm( 41.14663)

Phase\_Density\_g\_on\_cm3( 1.57425)

a 14.78794\_0.00076

b 4.82142\_0.00020

c 19.87957\_0.00071

be 120.97069\_0.00481

RB\_2

...

xdd a\_CPC\_250C010224.xy

bkg @ 2380.98011` -69.3822272` 12.892117` -20.5822191` -17.6006265` 10.1386738` -5.55179119`  
16.0163999` -21.7186642` -7.25870792` 0.0162196701`

information

str space\_group P-1  
r\_bragg 0.649266627

prm scale\_a224 = -(scale\_b224\*mb\*vb\*(Exp(-((k\*t224)^n)))/(ma\*va\*((Exp(-((k\*t224)^n))-1))));:0.00002`  
scale =scale\_a224;: 0.0000199555`

phase\_name a-cpc

cell\_mass 576.081

cell\_volume 605.1501

weight\_percent wa224 2.394

Phase\_LAC\_1\_on\_cm( 41.31710)

Phase\_Density\_g\_on\_cm3( 1.58077)

CS\_G(, 25.10749\_0.33412)

Strain\_L(, 2.62461\_0.07480)

Out(wa224, " Anteil\_a224:\ %11.5f","error:\t%11.5f")

Out(scale\_a224, " Skalierung\_a224:\%11.5f","error:\t%11.5f")

a 3.83112\_0.00166  
b 13.03000\_0.00149  
c 12.21495\_0.00210  
a1 88.99493\_0.03895  
be 96.95233\_0.05200  
ga 89.48921\_0.06164

RB\_1

str CS\_G(, 132.20025\_4.32425)  
Strain\_L(, 0.36128\_0.00985)  
r\_bragg 0.655795854  
phase\_name b-cpc  
cell\_mass 1152.162  
cell\_volume 1215.3144

weight\_percent wb224 97.606

scale =scale\_b224;:0.0002025588`

Out(wb224, " Anteil\_b224:\ %11.5f","error:\t%11.5f")

Out(scale\_b224, " Skalierung\_b224:\%11.5f","error:\t%11.5f\n")

space\_group P21/c  
Phase\_LAC\_1\_on\_cm( 41.14663)  
Phase\_Density\_g\_on\_cm3( 1.57425)

a 14.78794\_0.00076  
b 4.82142\_0.00020  
c 19.87957\_0.00071  
  
be 120.97069\_0.00481

RB\_2