

Inp-File for parametric refinement of non-isothermal measurement

```
prn !D 143.25982
prn !PSF 0.15373
prn !d 0.16530
prn !mix 0.00000_LIMIT_MIN_0 min 0.0 max 1.0
gauss_fwhm = (1-mix) (ArcTan((D*Tan(2*Th)+PSF+d*(1/Cos(2*Th)))/D)-(2*Th))/Deg + 0.000001;

out "Version_6.txt " append

do_errors

macro information {

    start_X 2.5
    finish_X 30.0
    Zero_Error(, -0.02902_0.00041)
    LP_Factor( 90)
    convolution_step 2
    Rp 100
    Rs 100
    lam

        ymin_on_ymax 0.0001
        la 1 lo 0.922164 lh 1e-006
    x_calculation_step 0.02
}

prn scale_b1 0.00000`_0.00000_LIMIT_MIN_5.683e-007 min 0.0000005683 max 1
prn scale_b2 0.00000`_0.00000 min 0.0000005683 max 1
prn scale_b3 0.00000`_0.00000 min 0.0000005683 max 1
prn scale_b4 0.00001`_0.00000 min 0.0000005683 max 1
prn scale_b5 0.00001`_0.00000 min 0.0000005683 max 1
prn scale_b6 0.00003`_0.00000
prn scale_b7 0.00004`_0.00000
prn scale_b8 0.00006`_0.00000
prn scale_b9 0.00008`_0.00000
prn scale_b10 0.00009`_0.00000
prn scale_b11 0.00010`_0.00000

prn !t1 515
prn !t2 520
prn !t3 525
prn !t4 530
prn !t5 535
prn !t6 540
prn !t7 545
prn !t8 550
prn !t9 555
prn !t10 560
```

prm !t11 565

prm c 76.86917`_0.26927

prm !n 1.5

prm !r 8.314

prm E 245007.30356`_774.85410

xdd pb15_INDEX_7519.xy

bkg @ 1499.09295`_2.34111297 -215.462663`_3.2856927 -126.45465`_2.83487757
172.451498`_2.61760539 22.0787092`_2.78467922 -70.286256`_2.64118778 -28.3586458`_2.76756045
74.29406`_2.60444284 -2.19303067`_2.55981989 -30.0373477`_2.38593468 10.5230583`_2.25985824
25.9365424`_2.30263817 -17.8482526`_2.26335159 -2.28252527`_2.23587168

information

str CS_G(, 38.08542_1.47016)
Strain_L(, 1.59343_0.06067)
CS_L(, 55.52277_3.05829)

r_bragg 1.20098865
phase_name a-cpc
cell_mass ma1 576.081_0.000
cell_volume va1 602.1848_0.0000
weight_percent wa1 99.484_0.201

prm x11 =c+n*3.5836-1.052*n*E/(r*t1);:-8.05148`_0.39250
prm x21 =Exp(-Exp(x11));:0.99968`_0.00013
prm scale_a1 =(-x21*ma1*va1*scale_b1)/((x21-1)*vb1*mb1);:0.00044`_0.00017
scale =scale_a1;:0.0004420735`_0.0000000000
space_group P-1
Phase_LAC_1_on_cm(22.73093_0.00000)
Phase_Density_g_on_cm3(1.58856_0.00000)

Out(wa1, " Anteil_a1:\ %11.5f", "error:\t%11.5f")

a 3.83957_0.00152
b 12.98271_0.00153
c 12.15789_0.00199
a1 89.13055_0.02883
be 96.40412_0.04737
ga 89.75451_0.04919

prm Bov1 10.20287`_0.26161 min 0 max 20

site Cu41 x 0.00000_0.00000 y 0.00000_0.00000 z 0.00000_0.00000 occ Cu 1 beq=Bov1;
site N4 x -0.05894_0.00000 y 0.13797_0.00000 z -0.07505_0.00000 occ N 1 beq=Bov1;
site N10 x 0.26598_0.00000 y 0.06438_0.00000 z 0.13166_0.00000 occ N 1 beq=Bov1;
site C2 x -0.22912_0.00000 y 0.15729_0.00000 z -0.17753_0.00000 occ C 1 beq=Bov1;

site C5 x 0.06449_0.00000 y 0.22825_0.00000 z -0.03215_0.00000 occ C 1 beq=Bov1;
 site C11 x 0.40419_0.00000 y 0.01384_0.00000 z 0.22539_0.00000 occ C 1 beq=Bov1;
 site C12 x 0.33930_0.00000 y 0.16602_0.00000 z 0.14268_0.00000 occ C 1 beq=Bov1;
 site C1 x -0.21488_0.00000 y 0.26289_0.00000 z -0.20126_0.00000 occ C 1 beq=Bov1;
 site C3 x -0.02895_0.00000 y 0.30816_0.00000 z -0.10931_0.00000 occ C 1 beq=Bov1;
 site N39 x 0.24799_0.00000 y 0.24211_0.00000 z 0.06789_0.00000 occ N 1 beq=Bov1;
 site C13 x 0.57100_0.00000 y 0.08480_0.00000 z 0.29875_0.00000 occ C 1 beq=Bov1;
 site N38 x 0.38880_0.00000 y -0.08805_0.00000 z 0.24735_0.00000 occ N 1 beq=Bov1;
 site C14 x 0.52990_0.00000 y 0.18134_0.00000 z 0.24632_0.00000 occ C 1 beq=Bov1;
 site C6 x -0.34842_0.00000 y 0.32299_0.00000 z -0.29522_0.00000 occ C 1 beq=Bov1;
 site C8 x 0.03313_0.00000 y 0.41552_0.00000 z -0.10640_0.00000 occ C 1 beq=Bov1;
 site C15 x 0.75409_0.00000 y 0.07300_0.00000 z 0.40629_0.00000 occ C 1 beq=Bov1;
 site C17 x 0.67006_0.00000 y 0.27098_0.00000 z 0.29890_0.00000 occ C 1 beq=Bov1;
 site C7 x -0.28834_0.00000 y 0.43072_0.00000 z -0.29355_0.00000 occ C 1 beq=Bov1;
 site H42 x -0.48562_0.00000 y 0.28970_0.00000 z -0.36311_0.00000 occ H 1 beq=Bov1;
 site C9 x -0.09906_0.00000 y 0.47678_0.00000 z -0.19994_0.00000 occ C 1 beq=Bov1;
 site H44 x 0.17041_0.00000 y 0.44854_0.00000 z -0.03838_0.00000 occ H 1 beq=Bov1;
 site C16 x 0.89600_0.00000 y 0.16212_0.00000 z 0.46003_0.00000 occ C 1 beq=Bov1;
 site H46 x 0.78410_0.00000 y 0.00179_0.00000 z 0.44479_0.00000 occ H 1 beq=Bov1;
 site C18 x 0.85430_0.00000 y 0.26041_0.00000 z 0.40673_0.00000 occ C 1 beq=Bov1;
 site H48 x 0.63985_0.00000 y 0.34213_0.00000 z 0.26030_0.00000 occ H 1 beq=Bov1;
 site H43 x -0.38286_0.00000 y 0.47595_0.00000 z -0.36087_0.00000 occ H 1 beq=Bov1;
 site H45 x -0.05724_0.00000 y 0.55498_0.00000 z -0.19975_0.00000 occ H 1 beq=Bov1;
 site H47 x 1.03006_0.00000 y 0.15547_0.00000 z 0.53818_0.00000 occ H 1 beq=Bov1;
 site H49 x 0.95847_0.00000 y 0.32445_0.00000 z 0.44660_0.00000 occ H 1 beq=Bov1;

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 -47.83577_0.06702 qa 1 operate_on_points "C* H* N* "
 rotate -234.99167_0.05432 qb 1 operate_on_points "C* H* N* "
 rotate 41.21788_0.07547 qc 1 operate_on_points "C* H* N* "

str Strain_G(, 0.44094_0.01275)

r_bragg 1.38451498
 phase_name b-cpc
 cell_mass mb1 1152.162_0.000
 cell_volume vb1 1214.5866_0.0000
 weight_percent wb1 0.516_0.201

scale =scale_b1;:0.0000005683`_0.0000000097
 space_group P21/c
 Phase_LAC_1_on_cm(22.53972_0.00000)
 Phase_Density_g_on_cm3(1.57519_0.00000)

Out(wb1, " Anteil_b1:\t %11.5f", "error:\t%11.5f\n")

a 14.77449_0.00082
 b 4.82504_0.00023
 c 19.87803_0.00081

be 121.00524_0.00504

site Cu41 x 0.00000_0.00000 y 0.00000_0.00000 z 0.00000_0.00000 occ Cu 1 beq=Bov1;
 site N4 x 0.07208_0.00000 y -0.21726_0.00000 z 0.09982_0.00000 occ N 1 beq=Bov1;
 site N10 x 0.13509_0.00000 y 0.19633_0.00000 z 0.03140_0.00000 occ N 1 beq=Bov1;
 site C2 x 0.02619_0.00000 y -0.41194_0.00000 z 0.12217_0.00000 occ C 1 beq=Bov1;
 site C5 x 0.17525_0.00000 y -0.19509_0.00000 z 0.15676_0.00000 occ C 1 beq=Bov1;
 site C11 x 0.14901_0.00000 y 0.39421_0.00000 z -0.01119_0.00000 occ C 1 beq=Bov1;
 site C12 x 0.22855_0.00000 y 0.15470_0.00000 z 0.09891_0.00000 occ C 1 beq=Bov1;
 site C1 x 0.10188_0.00000 y -0.51802_0.00000 z 0.19550_0.00000 occ C 1 beq=Bov1;
 site C3 x 0.19649_0.00000 y -0.38108_0.00000 z 0.21764_0.00000 occ C 1 beq=Bov1;
 site N39 x 0.24798_0.00000 y -0.02477_0.00000 z 0.15700_0.00000 occ N 1 beq=Bov1;
 site C13 x 0.25423_0.00000 y 0.48244_0.00000 z 0.02996_0.00000 occ C 1 beq=Bov1;
 site N38 x 0.07541_0.00000 y 0.49489_0.00000 z -0.08186_0.00000 occ N 1 beq=Bov1;
 site C14 x 0.30471_0.00000 y 0.33057_0.00000 z 0.09980_0.00000 occ C 1 beq=Bov1;
 site C6 x 0.09599_0.00000 y -0.72207_0.00000 z 0.24456_0.00000 occ C 1 beq=Bov1;
 site C8 x 0.28990_0.00000 y -0.44064_0.00000 z 0.28973_0.00000 occ C 1 beq=Bov1;

```

site C15  x  0.30961_0.00000 y  0.68163_0.00000 z  0.01222_0.00000 occ C 1 beq=Bov1;
site C17  x  0.41323_0.00000 y  0.37042_0.00000 z  0.15543_0.00000 occ C 1 beq=Bov1;
site C7   x  0.18895_0.00000 y -0.78408_0.00000 z  0.31701_0.00000 occ C 1 beq=Bov1;
site H42  x  0.02625_0.00000 y -0.82325_0.00000 z  0.22830_0.00000 occ H 1 beq=Bov1;
site C9   x  0.28525_0.00000 y -0.64465_0.00000 z  0.33954_0.00000 occ C 1 beq=Bov1;
site H44  x  0.35949_0.00000 y -0.33907_0.00000 z  0.30580_0.00000 occ H 1 beq=Bov1;
site C16  x  0.41840_0.00000 y  0.72386_0.00000 z  0.06739_0.00000 occ C 1 beq=Bov1;
site H46  x  0.27227_0.00000 y  0.79335_0.00000 z -0.03928_0.00000 occ H 1 beq=Bov1;
site C18  x  0.46985_0.00000 y  0.56938_0.00000 z  0.13849_0.00000 occ C 1 beq=Bov1;
site H48  x  0.45047_0.00000 y  0.25858_0.00000 z  0.20689_0.00000 occ H 1 beq=Bov1;
site H43  x  0.18658_0.00000 y -0.93159_0.00000 z  0.35362_0.00000 occ H 1 beq=Bov1;
site H45  x  0.35211_0.00000 y -0.69149_0.00000 z  0.39222_0.00000 occ H 1 beq=Bov1;
site H47  x  0.46029_0.00000 y  0.86745_0.00000 z  0.05580_0.00000 occ H 1 beq=Bov1;
site H49  x  0.54877_0.00000 y  0.60197_0.00000 z  0.17802_0.00000 occ H 1 beq=Bov1;

```

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 -222.83750_0.03028 min -237 max -207 qa 1 operate_on_points "C* H* N* "
rotate -199.45467_0.03986 min -214 max -184 qb 1 operate_on_points "C* H* N* "
rotate  28.86274_0.05554 min  13 max  43 qc 1 operate_on_points "C* H* N* "

```

...

xdd pb15_INDEX_9309.xy

bkg @ 1465.04176`_1.74125814 -197.290127`_2.87830108 -138.748818`_2.62356098
167.476045`_2.5321154 -4.27435284`_2.46510311 -64.646383`_2.46155211 -27.5080852`_2.40568045
71.9367942`_2.37030611 -30.8263922`_2.28434085 -13.2018889`_2.27341191 13.4519512`_2.16134365
13.1401499`_2.15726675 -30.9426973`_1.97032202 16.9594178`_1.9775273

information

str CS_G(, 41.72758_3.53940)
Strain_L(, 1.18637_0.07252)
CS_L(, 64.62458_7.43804)

r_bragg 0.957471981
phase_name a-cpc
cell_mass ma11 576.081_0.000
cell_volume va11 607.7636_0.0000
weight_percent wa11 3.851_2.140

prm x111 =c+n*3.5836-1.052*n*E/(r*t11);: -0.06068`_0.37451
prm x211 =Exp(-Exp(x111));:0.39019`_0.13753
prm scale_a11 =(-x211*ma11*va11*scale_b11)/((x211-1)*vb11*mb11);:0.00002`_0.00001
scale =scale_a11;:0.0000158806`_0.0000000000
space_group P-1
Phase_LAC_1_on_cm(22.52228_0.00000)
Phase_Density_g_on_cm3(1.57398_0.00000)

Out(wa11, " Anteil_a11:\t %11.5f", "error:\t%11.5f")

a 3.864534_0.01350
b 13.03595_0.01275
c 12.13906_0.01147
a1 89.38399_0.21934
be 96.30929_0.37610
ga 89.43683_0.34570

prm Bov11 8.13912`_0.13822 min 0 max 20

site Cu41 x 0.00000_0.00000 y 0.00000_0.00000 z 0.00000_0.00000 occ Cu 1

beq=Bov11;

site N4 x -0.06278_0.00000 y 0.13704_0.00000 z -0.07529_0.00000 occ N 1 beq=Bov11;
site N10 x 0.26652_0.00000 y 0.06474_0.00000 z 0.13098_0.00000 occ N 1 beq=Bov11;
site C2 x -0.23478_0.00000 y 0.15578_0.00000 z -0.17749_0.00000 occ C 1 beq=Bov11;
site C5 x 0.05943_0.00000 y 0.22715_0.00000 z -0.03287_0.00000 occ C 1 beq=Bov11;
site C11 x 0.40706_0.00000 y 0.01487_0.00000 z 0.22457_0.00000 occ C 1 beq=Bov11;

site C12 x 0.33794_0.00000 y 0.16602_0.00000 z 0.14159_0.00000 occ C 1 beq=Bov11;
 site C1 x -0.22302_0.00000 y 0.26083_0.00000 z -0.20153_0.00000 occ C 1 beq=Bov11;
 site C3 x -0.03672_0.00000 y 0.30635_0.00000 z -0.11005_0.00000 occ C 1 beq=Bov11;
 site N39 x 0.24405_0.00000 y 0.24143_0.00000 z 0.06678_0.00000 occ N 1 beq=Bov11;
 site C13 x 0.57347_0.00000 y 0.08588_0.00000 z 0.29742_0.00000 occ C 1 beq=Bov11;
 site N38 x 0.39404_0.00000 y -0.08650_0.00000 z 0.24683_0.00000 occ N 1 beq=Bov11;
 site C14 x 0.52968_0.00000 y 0.18176_0.00000 z 0.24482_0.00000 occ C 1 beq=Bov11;
 site C6 x -0.35909_0.00000 y 0.32023_0.00000 z -0.29538_0.00000 occ C 1 beq=Bov11;
 site C8 x 0.02324_0.00000 y 0.41328_0.00000 z -0.10754_0.00000 occ C 1 beq=Bov11;
 site C15 x 0.75830_0.00000 y 0.07464_0.00000 z 0.40463_0.00000 occ C 1 beq=Bov11;
 site C17 x 0.66876_0.00000 y 0.27128_0.00000 z 0.29690_0.00000 occ C 1 beq=Bov11;
 site C7 x -0.30116_0.00000 y 0.42752_0.00000 z -0.29411_0.00000 occ C 1 beq=Bov11;
 site H42 x -0.49656_0.00000 y 0.28675_0.00000 z -0.36292_0.00000 occ H 1 beq=Bov11;
 site C9 x -0.11150_0.00000 y 0.47384_0.00000 z -0.20098_0.00000 occ C 1 beq=Bov11;
 site H44 x 0.16080_0.00000 y 0.44649_0.00000 z -0.03988_0.00000 occ H 1 beq=Bov11;
 site C16 x 0.89916_0.00000 y 0.16365_0.00000 z 0.45787_0.00000 occ C 1 beq=Bov11;
 site H46 x 0.79029_0.00000 y 0.00391_0.00000 z 0.44327_0.00000 occ H 1 beq=Bov11;
 site C18 x 0.85473_0.00000 y 0.26128_0.00000 z 0.40439_0.00000 occ C 1 beq=Bov11;
 site H48 x 0.63657_0.00000 y 0.34195_0.00000 z 0.25817_0.00000 occ H 1 beq=Bov11;
 site H43 x -0.39753_0.00000 y 0.47224_0.00000 z -0.36136_0.00000 occ H 1 beq=Bov11;
 site H45 x -0.07126_0.00000 y 0.55171_0.00000 z -0.20108_0.00000 occ H 1 beq=Bov11;
 site H47 x 1.03445_0.00000 y 0.15740_0.00000 z 0.53577_0.00000 occ H 1 beq=Bov11;
 site H49 x 0.95816_0.00000 y 0.32524_0.00000 z 0.44389_0.00000 occ H 1 beq=Bov11;

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 -47.98896_0.14280 qa 1 operate_on_points "C* H* N* "
rotate -234.31097_0.11182 qb 1 operate_on_points "C* H* N* "
rotate 41.58749_0.16825 qc 1 operate_on_points "C* H* N* "

str Strain_G(, 0.44094_0.01275)

r_bragg 1.44952666
phase_name b-cpc
cell_mass mb11 1152.162_0.000
cell_volume vb11 1214.5866_0.0000
weight_percent wb11 96.149_2.140

scale =scale_b11;:0.0000991995`_0.0000002962
space_group P21/c
Phase_LAC_1_on_cm( 22.53972_0.00000)
Phase_Density_g_on_cm3( 1.57519_0.00000)

Out(wb11, " Anteil_b11:\ %11.5f", "error:\t%11.5f\n")

a 14.77449_0.00082
b 4.82504_0.00023
c 19.87803_0.00081

be 121.00524_0.00504

site Cu41 x 0.00000_0.00000 y 0.00000_0.00000 z 0.00000_0.00000 occ Cu 1
beq=Bov11;

site N4 x 0.07208_0.00000 y -0.21726_0.00000 z 0.09982_0.00000 occ N 1 beq=Bov11;
site N10 x 0.13509_0.00000 y 0.19633_0.00000 z 0.03140_0.00000 occ N 1 beq=Bov11;
site C2 x 0.02619_0.00000 y -0.41194_0.00000 z 0.12217_0.00000 occ C 1 beq=Bov11;
site C5 x 0.17525_0.00000 y -0.19509_0.00000 z 0.15676_0.00000 occ C 1 beq=Bov11;
site C11 x 0.14901_0.00000 y 0.39421_0.00000 z -0.01119_0.00000 occ C 1 beq=Bov11;
site C12 x 0.22855_0.00000 y 0.15470_0.00000 z 0.09891_0.00000 occ C 1 beq=Bov11;
site C1 x 0.10188_0.00000 y -0.51802_0.00000 z 0.19550_0.00000 occ C 1 beq=Bov11;
site C3 x 0.19649_0.00000 y -0.38108_0.00000 z 0.21764_0.00000 occ C 1 beq=Bov11;
site N39 x 0.24798_0.00000 y -0.02477_0.00000 z 0.15700_0.00000 occ N 1 beq=Bov11;
site C13 x 0.25423_0.00000 y 0.48244_0.00000 z 0.02996_0.00000 occ C 1 beq=Bov11;
site N38 x 0.07541_0.00000 y 0.49489_0.00000 z -0.08186_0.00000 occ N 1 beq=Bov11;
site C14 x 0.30471_0.00000 y 0.33057_0.00000 z 0.09980_0.00000 occ C 1 beq=Bov11;
site C6 x 0.09599_0.00000 y -0.72207_0.00000 z 0.24456_0.00000 occ C 1 beq=Bov11;
site C8 x 0.28990_0.00000 y -0.44064_0.00000 z 0.28973_0.00000 occ C 1 beq=Bov11;
site C15 x 0.30961_0.00000 y 0.68163_0.00000 z 0.01222_0.00000 occ C 1 beq=Bov11;
site C17 x 0.41323_0.00000 y 0.37042_0.00000 z 0.15543_0.00000 occ C 1 beq=Bov11;

```

site C7 x 0.18895_0.00000 y -0.78408_0.00000 z 0.31701_0.00000 occ C 1 beq=Bov11;
 site H42 x 0.02625_0.00000 y -0.82325_0.00000 z 0.22830_0.00000 occ H 1 beq=Bov11;
 site C9 x 0.28525_0.00000 y -0.64465_0.00000 z 0.33954_0.00000 occ C 1 beq=Bov11;
 site H44 x 0.35949_0.00000 y -0.33907_0.00000 z 0.30580_0.00000 occ H 1 beq=Bov11;
 site C16 x 0.41840_0.00000 y 0.72386_0.00000 z 0.06739_0.00000 occ C 1 beq=Bov11;
 site H46 x 0.27227_0.00000 y 0.79335_0.00000 z -0.03928_0.00000 occ H 1 beq=Bov11;
 site C18 x 0.46985_0.00000 y 0.56938_0.00000 z 0.13849_0.00000 occ C 1 beq=Bov11;
 site H48 x 0.45047_0.00000 y 0.25858_0.00000 z 0.20689_0.00000 occ H 1 beq=Bov11;
 site H43 x 0.18658_0.00000 y -0.93159_0.00000 z 0.35362_0.00000 occ H 1 beq=Bov11;
 site H45 x 0.35211_0.00000 y -0.69149_0.00000 z 0.39222_0.00000 occ H 1 beq=Bov11;
 site H47 x 0.46029_0.00000 y 0.86745_0.00000 z 0.05580_0.00000 occ H 1 beq=Bov11;
 site H49 x 0.54877_0.00000 y 0.60197_0.00000 z 0.17802_0.00000 occ H 1 beq=Bov11;

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 -222.83750_0.03028 min -237 max -207 qa 1 operate_on_points "C* H* N* "

rotate -199.45467_0.03986 min -214 max -184 qb 1 operate_on_points "C* H* N* "

rotate 28.86274_0.05554 min 13 max 43 qc 1 operate_on_points "C* H* N* "