Supporting information

for article

Parameterization of the coupling between strain and order parameter for $LuF[SeO_3]$

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Section S1. Calculation of the strain components.

For calculations of the strains the following formulas were used (Carpenter *et al.*, 1998):

$$e_1 = \frac{a}{a_0}\sin\gamma - 1$$

$$e_2 = \frac{b}{b_0} - 1$$

$$e_3 = \frac{c\sin\alpha\sin\beta^*}{c_0\sin\beta_0^*} - 1$$

$$e_4 = \frac{c\cos\alpha}{c_0\sin\beta_0^*} + \frac{a\cos\beta_0^*\cos\gamma}{a_0\sin\beta_0^*}$$

$$e_5 = \frac{a\sin\gamma\cos\beta_0^*}{a_0\sin\beta_0^*} - \frac{c\sin\alpha\cos\beta^*}{c_0\sin\beta_0^*}$$

$$e_6 = \frac{a}{a_0}\cos\gamma$$

Asterics (*) refers to the reciprocal lattice angles.

Section S2. Simulated heating/cooling-Guinier pattern.

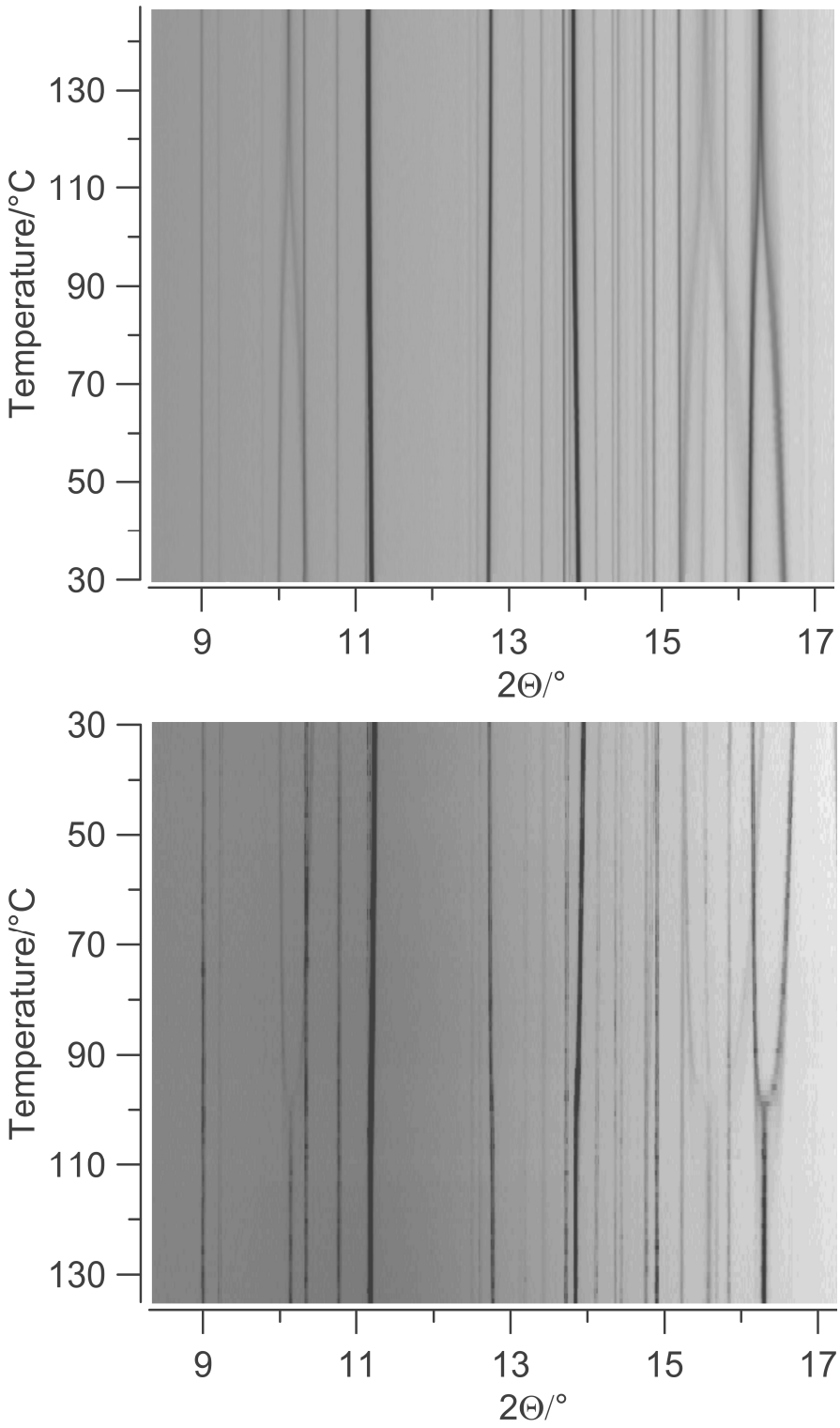

Fig. S2. Two-dimensional projection (simulated heating/cooling-Guinier pattern, prepared using Powder3D (Hinrichsen *et al.*, 2006)) of the observed scattered X-ray intensity for $LuF[SeO_3]$ as a function of diffraction angle (x-axis) and temperature (*y*-axis), top – on heating, bottom – on cooling.

Section S3. Temperature dependence of symmetry-adapted strains for $LuF[SeO_3]$.

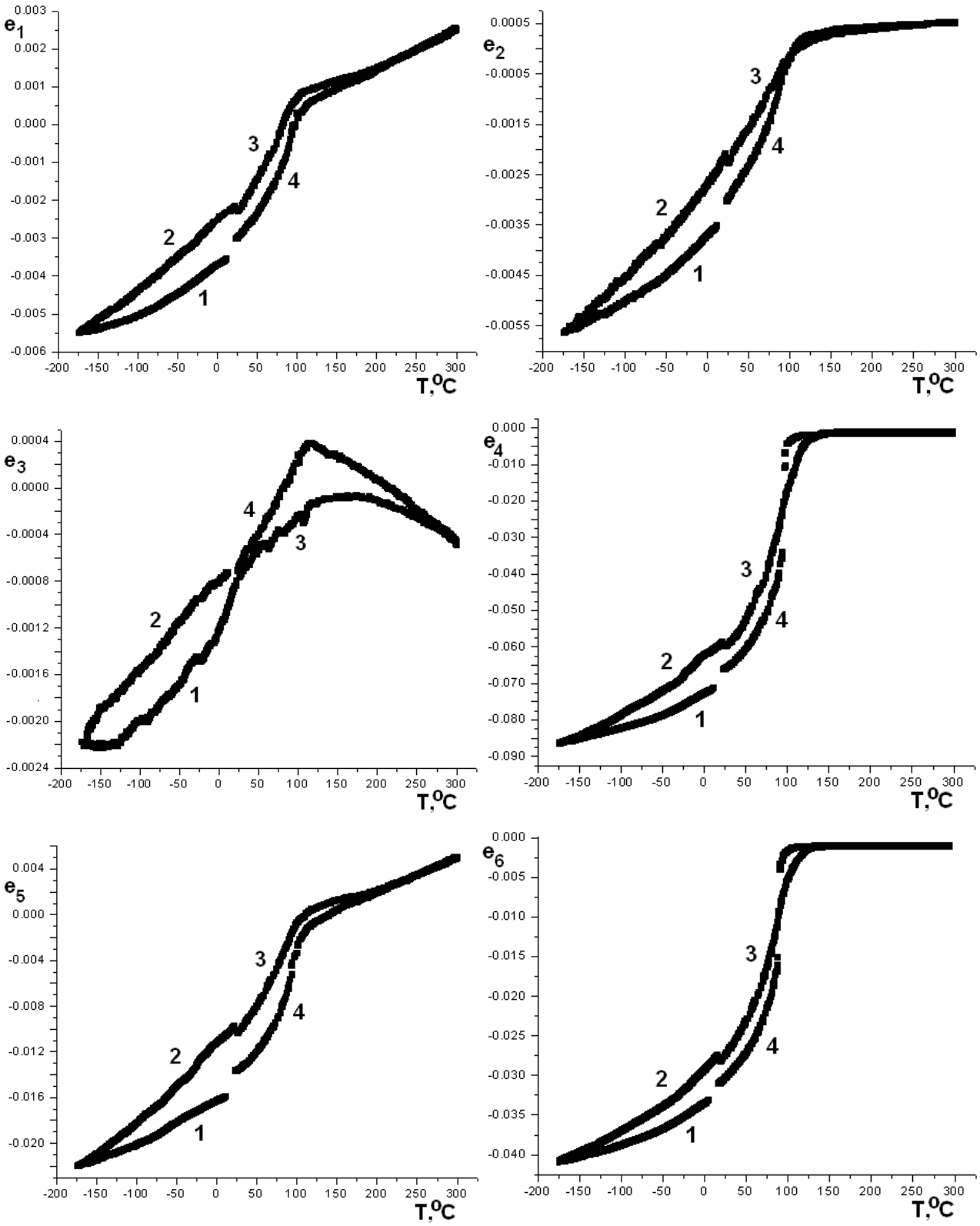

Fig. S3. Temperature dependence of symmetry-adapted strains for $LuF[SeO_3]$. Numbers show the sequence of cooling and heating: 1 – cooling from RT to -173°C, 2 – heating from -173°C to RT, 3 – heating from RT to 300°C, 4 – cooling from 300°C to RT.

Unit cell dimensions at RT before cooling (at the begin of step 1): 6.4504(1); 6.8460(1); 4.2812(1); 94.084(2); 96.509(2); 91.899(2); at RT after cooling (at the end of step 2): 6.4594(1); 6.8558(1); 4.2808(1); 93.364(3); 96.159(3); 91.574(2); at RT before heating (at the begin of step 3): 6.4586(1); 6.8545(1); 4.2810(1); 93.435(2); 96.174(2); 91.615(2); at RT after cooling (at the end of step 4): 6.4549(1); 6.8508(1); 4.2815(1); 93.690(3); 96.382(2); 91.711(1).

Section S4. Example of an input file for program Topas 4 which was used for the sequential Rietveld fit of the strain modes for $LuF[SeO_3]$.

```
macro Out_file(file)
{
   out file append
      Out(Get(r_wp), "    \n %11.5f" ) ' _Rwp
      Out(Get(a), "%15.5f", "%9.5f") ' cell_length_a
      Out(Get(b), "%15.5f", "%9.5f") ' cell_length_b
      Out(Get(c), "%15.5f", "%9.5f") ' cell_length_c
      Out(Get(al), "%15.5f", "%9.5f") ' cell_angle_alpha
      Out(Get(be), "%15.5f", "%9.5f") ' cell_angle_beta
      Out(Get(ga), "%15.5f", "%9.5f") ' cell_angle_gamma
      Out(s1, "%12.5f", "%9.5f")
      Out(s2, "%12.5f", "%9.5f")
      Out(s3, "%12.5f", "%9.5f")
      Out(s4, "%12.5f", "%9.5f")
      Out(s5, "%12.5f", "%9.5f")
      Out(s6, "%12.5f", "%9.5f")
      Out(pe1, "%12.5f", "%9.5f")
      Out(pe2, "%12.5f", "%9.5f")
      Out(pe3, "%12.5f", "%9.5f")
      Out(pe4, "%12.5f", "%9.5f")
      Out(pe5, "%12.5f", "%9.5f")
      Out(pe6, "%12.5f", "%9.5f")
}

'{{{macros for calculations involving the lattice parameters

      'Takes non-refinable undistorted cell parameters, and variable strains as
input.
      'Returns strained cell parameters
      macro straincell(pa0, pb0, pc0, pal0, pbe0, pga0)
      {
            prm  !radian  57.2957795
            prm  palpha0 = pal0/radian;
            prm  pbeta0  = pbe0/radian;
            prm  pgamma0 = pga0/radian;
            'distorted parent-cell parameters
            prm  pa = pa0*(pe1 + 1);:  6.44848
            prm  pb = pb0*(pe2 + 1);:  6.84409
            prm  pc = pc0*(pe3 + 1);:  4.27980
            prm  palpha = palpha0 - pe4*Sin(palpha0);
            prm  pbeta  = pbeta0  - pe5*Sin(pbeta0);
            prm  pgamma = pgamma0 - pe6*Sin(pgamma0);
            prm  pal = palpha*radian;: 90.07091
            prm  pbe = pbeta*radian ;: 95.61740
            prm  pga = pgamma*radian;: 90.03307
      }

      'Use basis-transformation matrix to transform from parent-cell to supercell
parameters
      macro celltransform(t11, t12, t13, t21, t22, t23, t31, t32, t33)
      {
            prm  !radian  57.2957795

            'parent-lattice basis vectors in cartesian coords
            prm  zzz  = (Cos(palpha) - Cos(pbeta)*Cos(pgamma))/Sin(pgamma);
            prm  pv11 = pa;
            prm  !pv21  0
            prm  !pv31  0
```

```
            prm  pv12 = pb*Cos(pgamma);
            prm  pv22 = pb*Sin(pgamma);
            prm  !pv32  0
            prm  pv13 = pc*Cos(pbeta);
            prm  pv23 = pc*zzz;
            prm  pv33 = pc*Sqrt(1 - Cos(pbeta)^2 - zzz^2);

            'supercell basis vectors in cartesian coords
            prm  sv11 = t11*pv11 + t12*pv12 + t13*pv13;
            prm  sv21 = t11*pv21 + t12*pv22 + t13*pv23;
            prm  sv31 = t11*pv31 + t12*pv32 + t13*pv33;
            prm  sv12 = t21*pv11 + t22*pv12 + t23*pv13;
            prm  sv22 = t21*pv21 + t22*pv22 + t23*pv23;
            prm  sv32 = t21*pv31 + t22*pv32 + t23*pv33;
            prm  sv13 = t31*pv11 + t32*pv12 + t33*pv13;
            prm  sv23 = t31*pv21 + t32*pv22 + t33*pv23;
            prm  sv33 = t31*pv31 + t32*pv32 + t33*pv33;

            'distorted supercell parameters
            prm  sa = Sqrt(sv11^2+sv21^2+sv31^2);
            prm  sb = Sqrt(sv12^2+sv22^2+sv32^2);
            prm  sc = Sqrt(sv13^2+sv23^2+sv33^2);
            prm  salpha = ArcCos((sv12*sv13+sv22*sv23+sv32*sv33)/(sb*sc));
            prm  sbeta  = ArcCos((sv11*sv13+sv21*sv23+sv31*sv33)/(sa*sc));
            prm  sgamma = ArcCos((sv11*sv12+sv21*sv22+sv31*sv32)/(sa*sb));
            prm  sal = salpha*radian;
            prm  sbe = sbeta*radian;
            prm  sga = sgamma*radian;
      }
'}}}

iters 300
do_errors
XYE(FileName)
bkg @  11753.9469`_14.7944678 -7130.01235`_25.1300073  1935.93213`_23.0003751
561.944125`_21.3053992 -368.916997`_20.9094482  35.1972098`_19.8681934 -
24.8299646`_19.7882956  149.933676`_18.4599147  119.144117`_18.3542657
90.609349`_15.9106356 -52.0456283`_15.1624355
      start_X  4
      finish_X  30
      LP_Factor( 90)
      Zero_Error(, -0.0138)
      convolution_step 5
      Rp 217.5
      Rs 217.5
      Simple_Axial_Model( 0.001)
      lam
            ymin_on_ymax  0.0001
            la  1 lo  0.826401 lh  0.0001
      x_calculation_step 0.001
      str
            LVol_FWHM_CS_G_L( 1, 371.24214`_52.84462, 0.89, 358.49782`_45.08627,@,
411.79449`_49.86917,@, 9999.99999`_20342.19111)
            e0_from_Strain( 0.04488`_12.28008,lg, 0.17951`_0.00427,lg,
0.17951`_0.00427)
            r_bragg  6.55700305
            phase_name "Structure"
            MVW( 641.847, 187.946784`_0.00573257063, 100.000`_0.000)
            scale @  0.000567754063`_6.89e-006
            Phase_LAC_1_on_cm( 531.89653`_0.01622)
            Phase_Density_g_on_cm3( 5.67082`_0.00017)
```

```
            space_group P-1

            #define refine_strain_modes  'comment out this line for a traditional
supercell-parameter refinement.

      '     #ifdef refine_strain_modes
            prm  s1     -0.00230`_0.00002 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM1+(a)strain_1(a)
            prm  s2     -0.01046`_0.00005 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM1+(a)strain_2(a)
            prm  s3     -0.00231`_0.00002 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM1+(a)strain_3(a)
            prm  s4     -0.00080`_0.00001 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM1+(a)strain_4(a)
            prm  s5     -0.02823`_0.00004 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM2+(a)strain_1(a)
            prm  s6     -0.06016`_0.00006 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM2+(a)strain_2(a)

            'unitless parent cell strains (in lattice rather than orthogonal
coords)
            prm  pe1      = +  1.00000*s1;: -0.00230`_0.00002
            prm  pe2      = +  1.00000*s3;: -0.00231`_0.00002
            prm  pe3      = +  1.00000*s4;: -0.00080`_0.00001
            prm  pe4      = +  1.00000*s6;: -0.06016`_0.00006
            prm  pe5      = +  1.00000*s2;: -0.01046`_0.00005
            prm  pe6      = +  1.00000*s5;: -0.02823`_0.00004

            straincell(6.47340,6.87020,4.28430,90.00000,95.60200,90.00000)
            celltransform(1,0,0,0,1,0,0,0,1)

                  a  = sa;:    6.45854`_0.00013
                  b  = sb;:    6.85435`_0.00012
                  c  = sc;:    4.28088`_0.00007
                  al = sal;:  93.44678`_0.00326
                  be = sbe;:  96.19830`_0.00258
                  ga = sga;:  91.61764`_0.00237

'{{{mode definitions
            prm  !a1     -0.01000 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM1+(a)[Lu1:e]A'_1(a)
            prm  !a2     -0.01291 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM1+(a)[Lu1:e]A'_2(a)
            prm  a3     -0.02820`_0.01233 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM2+(a)[Lu1:e]A''(a)
            prm  !a4     -0.02302 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM1+(a)[F1:e]A'_1(a)
            prm  !a5     -0.06958 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM1+(a)[F1:e]A'_2(a)
            prm  a6      0.07997`_0.07392 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM2+(a)[F1:e]A''(a)
            prm  !a7     -0.00079 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM1+(a)[Se1:e]A'_1(a)
            prm  !a8      0.03442 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM1+(a)[Se1:e]A'_2(a)
            prm  a9      0.18568`_0.02063 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM2+(a)[Se1:e]A''(a)
            prm  !a10    -0.03090 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM1+(a)[O1:e]A'_1(a)
            prm  !a11    -0.04852 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM1+(a)[O1:e]A'_2(a)
```

```
            prm  a12     0.23911`_0.05407 min  -1.41 max  1.41
'P2_1/m[0,0,0]GM2+(a)[O1:e]A''(a)
            prm  !a13    -0.06769 min  -2.00 max  2.00
'P2_1/m[0,0,0]GM1+(a)[O2:f]A_1(a)
            prm  !a14    -0.00842 min  -2.00 max  2.00
'P2_1/m[0,0,0]GM1+(a)[O2:f]A_2(a)
            prm  !a15    -0.02061 min  -2.00 max  2.00
'P2_1/m[0,0,0]GM1+(a)[O2:f]A_3(a)
            prm  a16    -0.44042`_0.04677 min  -2.00 max  2.00
'P2_1/m[0,0,0]GM2+(a)[O2:f]A_1(a)
            prm  a17    -0.24993`_0.04396 min  -2.00 max  2.00
'P2_1/m[0,0,0]GM2+(a)[O2:f]A_2(a)
            prm  a18     0.18712`_0.08173 min  -2.00 max  2.00
'P2_1/m[0,0,0]GM2+(a)[O2:f]A_3(a)
'}}}

'{{{mode-amplitude to delta transformation
            prm  Lu1_dx   = +  0.10923*a2;: -0.00141
            prm  Lu1_dy   = +  0.10292*a3;: -0.00290`_0.00127
            prm  Lu1_dz   = +  0.16505*a1;: -0.00165
            prm  F1_dx    = +  0.10923*a5;: -0.00760
            prm  F1_dy    = +  0.10292*a6;:  0.00823`_0.00761
            prm  F1_dz    = +  0.16505*a4;: -0.00380
            prm  Se1_dx   = -  0.10923*a8;: -0.00376
            prm  Se1_dy   = -  0.10292*a9;: -0.01911`_0.00212
            prm  Se1_dz   = -  0.16505*a7;:  0.00013
            prm  O1_dx    = +  0.10923*a11;: -0.00530
            prm  O1_dy    = +  0.10292*a12;:  0.02461`_0.00557
            prm  O1_dz    = +  0.16505*a10;: -0.00510
            prm  O2_dx    = +  0.07724*a14 +  0.07724*a17;: -0.01995`_0.00340
            prm  O2_dy    = +  0.07278*a15 +  0.07278*a18;:  0.01212`_0.00595
            prm  O2_dz    = +  0.11671*a13 +  0.11671*a16;: -0.05930`_0.00546
            prm  O3_dx    = +  0.07724*a14 -  0.07724*a17;:  0.01865`_0.00340
            prm  O3_dy    = -  0.07278*a15 +  0.07278*a18;:  0.01512`_0.00595
            prm  O3_dz    = +  0.11671*a13 -  0.11671*a16;:  0.04350`_0.00546
 '}}}

'{{{distorted parameters
            prm  Lu1_x    =    0.36836 + Lu1_dx;:  0.36695
            prm  Lu1_y    = 1/4 + Lu1_dy;:  0.24710`_0.00127
            prm  Lu1_z    =    0.46083 + Lu1_dz;:  0.45918
            prm  F1_x     =    0.35790 + F1_dx;:  0.35030
            prm  F1_y     = 1/4 + F1_dy;:  0.25823`_0.00761
            prm  F1_z     =   -0.03820 + F1_dz;: -0.04200
            prm  Se1_x    =    0.14630 + Se1_dx;:  0.14254
            prm  Se1_y    = 3/4 + Se1_dy;:  0.73089`_0.00212
            prm  Se1_z    =    0.32170 + Se1_dz;:  0.32183
            prm  O1_x     =    0.02340 + O1_dx;:  0.01810
            prm  O1_y     = 1/4 + O1_dy;:  0.27461`_0.00557
            prm  O1_z     =    0.41130 + O1_dz;:  0.40620
            prm  O2_x     =    0.32160 + O2_dx;:  0.30165`_0.00340
            prm  O2_y     =    0.92560 + O2_dy;:  0.93772`_0.00595
            prm  O2_z     =    0.45060 + O2_dz;:  0.39130`_0.00546
            prm  O3_x     =    0.32160 + O3_dx;:  0.34025`_0.00340
            prm  O3_y     =    0.57440 + O3_dy;:  0.58952`_0.00595
            prm  O3_z     =    0.45060 + O3_dz;:  0.49410`_0.00546

            prm !Lu1_occ  = 1;:  1.00000
            prm !F1_occ   = 1;:  1.00000
            prm !Se1_occ  = 1;:  1.00000
            prm !O1_occ   = 1;:  1.00000
            prm !O2_occ   = 1;:  1.00000
```

```
            prm !O3_occ   = 1;:  1.00000
'}}}

'{{{mode-dependent sites
            site Lu1  x = Lu1_x;  y = Lu1_y;  z = Lu1_z;  occ Lu = Lu1_occ;  beq
reflu   3.0577`_0.1879 min =0.2 ;
            site F1   x = F1_x;   y = F1_y;   z = F1_z;   occ F  = F1_occ;   beq
reff    0.2000`_0.8350 min =0.2 ;
            site Se1  x = Se1_x;  y = Se1_y;  z = Se1_z;  occ Se = Se1_occ;  beq
refse   5.5362`_0.4056 min =0.2 ;
            site O1   x = O1_x;   y = O1_y;   z = O1_z;   occ O  = O1_occ;   beq
refo   0.2000`_0.6530 min =0.2 ;
            site O2   x = O2_x;   y = O2_y;   z = O2_z;   occ O  = O2_occ;   beq
refo   0.2000`_0.6530 min =0.2 ;
            site O3   x = O3_x;   y = O3_y;   z = O3_z;   occ O  = O3_occ;   beq
refo   0.2000`_0.6530 min =0.2 ;
'}}}
```

Section S5. Example of an input file for program Topas 4 which was used for the sequential Le Bail fit of the strain modes for $LuF[SeO_3]$.

```
macro Out_file(file)
{
   out file append
      Out(Get(r_wp), "    \n %11.5f" ) ' _Rwp
      Out(Get(a), "%15.5f", "%9.5f") ' cell_length_a
      Out(Get(b), "%15.5f", "%9.5f") ' cell_length_b
      Out(Get(c), "%15.5f", "%9.5f") ' cell_length_c
      Out(Get(al), "%15.5f", "%9.5f") ' cell_angle_alpha
      Out(Get(be), "%15.5f", "%9.5f") ' cell_angle_beta
      Out(Get(ga), "%15.5f", "%9.5f") ' cell_angle_gamma
      Out(pe1, "%15.5f", "%9.5f")
      Out(pe2, "%15.5f", "%9.5f")
      Out(pe3, "%15.5f", "%9.5f")
      Out(pe4, "%15.5f", "%9.5f")
      Out(pe5, "%15.5f", "%9.5f")
      Out(pe6, "%15.5f", "%9.5f")
}
      macro straincell(pa0, pb0, pc0, pal0, pbe0, pga0)
      {
            prm  !radian  57.2957795
            prm  palpha0 = pal0/radian;
            prm  pbeta0  = pbe0/radian;
            prm  pgamma0 = pga0/radian;
            'distorted parent-cell parameters
            prm  pa = pa0*(pe1 + 1);:  6.44848
            prm  pb = pb0*(pe2 + 1);:  6.84409
            prm  pc = pc0*(pe3 + 1);:  4.27980
            prm  palpha = palpha0 - pe4*Sin(palpha0);
            prm  pbeta  = pbeta0  - pe5*Sin(pbeta0);
            prm  pgamma = pgamma0 - pe6*Sin(pgamma0);
            prm  pal = palpha*radian;: 90.07091
            prm  pbe = pbeta*radian ;: 95.61740
            prm  pga = pgamma*radian;: 90.03307
      }
      macro celltransform(t11, t12, t13, t21, t22, t23, t31, t32, t33)
      {
            prm  !radian  57.2957795
            'parent-lattice basis vectors in cartesian coords
            prm  zzz  = (Cos(palpha) - Cos(pbeta)*Cos(pgamma))/Sin(pgamma);
```

```
            prm  pv11 = pa;
            prm  !pv21  0
            prm  !pv31  0
            prm  pv12 = pb*Cos(pgamma);
            prm  pv22 = pb*Sin(pgamma);
            prm  !pv32  0
            prm  pv13 = pc*Cos(pbeta);
            prm  pv23 = pc*zzz;
            prm  pv33 = pc*Sqrt(1 - Cos(pbeta)^2 - zzz^2);
            'supercell basis vectors in cartesian coords
            prm  sv11 = t11*pv11 + t12*pv12 + t13*pv13;
            prm  sv21 = t11*pv21 + t12*pv22 + t13*pv23;
            prm  sv31 = t11*pv31 + t12*pv32 + t13*pv33;
            prm  sv12 = t21*pv11 + t22*pv12 + t23*pv13;
            prm  sv22 = t21*pv21 + t22*pv22 + t23*pv23;
            prm  sv32 = t21*pv31 + t22*pv32 + t23*pv33;
            prm  sv13 = t31*pv11 + t32*pv12 + t33*pv13;
            prm  sv23 = t31*pv21 + t32*pv22 + t33*pv23;
            prm  sv33 = t31*pv31 + t32*pv32 + t33*pv33;
            'distorted supercell parameters
            prm  sa = Sqrt(sv11^2+sv21^2+sv31^2);
            prm  sb = Sqrt(sv12^2+sv22^2+sv32^2);
            prm  sc = Sqrt(sv13^2+sv23^2+sv33^2);
            prm  salpha = ArcCos((sv12*sv13+sv22*sv23+sv32*sv33)/(sb*sc));
            prm  sbeta  = ArcCos((sv11*sv13+sv21*sv23+sv31*sv33)/(sa*sc));
            prm  sgamma = ArcCos((sv11*sv12+sv21*sv22+sv31*sv32)/(sa*sb));
            prm  sal = salpha*radian;
            prm  sbe = sbeta*radian;
            prm  sga = sgamma*radian;
      }
iters 100
do_errors
continue_after_convergence
XYE(FileName)
      bkg @  11209.8127` -7332.04118`  2248.66707`  312.4385` -446.151343`
48.9687557`  92.0060604`  62.5305514` -97.8755136` -150.174412`  40.1732165`
      start_X  4
      LP_Factor( 90)
      Zero_Error(, -0.0138)
      convolution_step 5
      Rp 217.5
```

```
      Rs 217.5
      Simple_Axial_Model( 0.001)
      lam
            ymin_on_ymax  0.0001
            la  1 lo  0.826401 lh  0.0001
      x_calculation_step 0.001
      hkl_Is
            lebail  1
            LVol_FWHM_CS_G_L( 1, 317.8518953, 0.89, 306.0315349,@, 350.4475805,@,
10000_LIMIT_MIN_0.3)
            e0_from_Strain( 0.06714911244,lg, 0.1637203233,lg, 0.1637203233)
            r_bragg  0.462166152
            phase_name "hkl_P-1"
            space_group "P-1"
            hkl_m_d_th2 0 1 0 2 6.83792591 6.92873144 I  0.03167503434
            hkl_m_d_th2 1 0 0 2 6.41686535 7.38399029 I  3.883647208
            hkl_m_d_th2 1 -1 0 2 4.76291418 9.95375633 I  1.968085691
            hkl_m_d_th2 1 1 0 2 4.59972572 10.3078327 I  1.666087449
            hkl_m_d_th2 0 0 1 2 4.24731684 11.1657076 I  35.1017308
            hkl_m_d_th2 1 0 -1 2 3.73559332 12.7011623 I  14.973385
            hkl_m_d_th2 0 -1 1 2 3.71510625 12.7714939 I  0.5720678465
            hkl_m_d_th2 0 1 1 2 3.50958157 13.5227985 I  0.3002439841
            hkl_m_d_th2 0 2 0 2 3.41896296 13.8829575 I  41.48216495
            hkl_m_d_th2 1 0 1 2 3.37526488 14.0635958 I  0.02639934675
            hkl_m_d_th2 1 1 -1 2 3.32830381 14.263052 I  0.03559812789
            hkl_m_d_th2 1 -1 -1 2 3.2304616 14.6973915 I  0.05614762095
            hkl_m_d_th2 2 0 0 2 3.20843267 14.7988653 I  0.6354186041
            hkl_m_d_th2 1 -1 1 2 3.11277413 15.2563143 I  5.681631878
            hkl_m_d_th2 1 -2 0 2 3.0620892 15.5103836 I  3.931344037
            hkl_m_d_th2 1 2 0 2 2.97459078 15.9695597 I  0.2948419239
            hkl_m_d_th2 1 1 1 2 2.94725585 16.1186523 I  4.110764447
            hkl_m_d_th2 2 -1 0 2 2.94439578 16.1344128 I  31.8610824
            hkl_m_d_th2 2 1 0 2 2.86635399 16.5767517 I  21.50942402
            hkl_m_d_th2 0 -2 1 2 2.74983549 17.28442 I  10.92717352
            hkl_m_d_th2 2 0 -1 2 2.70705819 17.5596905 I  0.2522461304
            hkl_m_d_th2 0 2 1 2 2.58443761 18.399889 I  5.025544893
            hkl_m_d_th2 1 2 -1 2 2.56783724 18.5198841 I  4.494602893
            hkl_m_d_th2 2 1 -1 2 2.5264852 18.8257408 I  10.55444544
            hkl_m_d_th2 2 -1 -1 2 2.50760698 18.968771 I  8.191734326
            hkl_m_d_th2 1 -2 1 2 2.48906946 19.1113625 I  0.625480755
            hkl_m_d_th2 1 -2 -1 2 2.4787128 19.191967 I  6.415372667
```

```
hkl_m_d_th2 2 0 1 2 2.43472695 19.5420589 I  0.01653932826
hkl_m_d_th2 2 -2 0 2 2.38145709 19.9836235 I  0.1609160045
hkl_m_d_th2 2 -1 1 2 2.34062719 20.3358898 I  15.29571802
hkl_m_d_th2 1 2 1 2 2.32342339 20.4880867 I  0.2304624266
hkl_m_d_th2 2 2 0 2 2.29986286 20.7002735 I  0.6435761287
hkl_m_d_th2 0 3 0 2 2.27930856 20.8890305 I  2.133650791
hkl_m_d_th2 2 1 1 2 2.24942732 21.1696987 I  2.537921561
hkl_m_d_th2 1 -3 0 2 2.17188907 21.9346733 I  5.45092177
hkl_m_d_th2 3 0 0 2 2.13895512 22.2766914 I  13.74680978
hkl_m_d_th2 2 2 -1 2 2.13375187 22.3317127 I  1.011896311
hkl_m_d_th2 1 3 0 2 2.12456274 22.4295502 I  4.910475903
hkl_m_d_th2 0 0 2 2 2.12365842 22.4392262 I  14.32599399
hkl_m_d_th2 2 -2 -1 2 2.11111546 22.5742931 I  5.095830096
hkl_m_d_th2 1 0 -2 2 2.08558846 22.8542938 I  8.260360785
hkl_m_d_th2 0 -1 2 2 2.06554317 23.0791206 I  0.08161570324
hkl_m_d_th2 0 -3 1 2 2.06365323 23.1005478 I  0.6368514118
hkl_m_d_th2 3 -1 0 2 2.06203032 23.1189785 I  4.78373099
hkl_m_d_th2 2 -2 1 2 2.04490328 23.3153172 I  3.571661755
hkl_m_d_th2 1 1 -2 2 2.02383375 23.5615063 I  0.6194230323
hkl_m_d_th2 3 1 0 2 2.02139831 23.5903015 I  6.838058186
hkl_m_d_th2 3 0 -1 2 2.00067735 23.8381939 I  2.138912158
hkl_m_d_th2 0 1 2 2 1.99262273 23.9359741 I  0.05554895191
hkl_m_d_th2 1 3 -1 2 1.97712755 24.1263771 I  0.6722031757
hkl_m_d_th2 1 -1 -2 2 1.96710289 24.251194 I  1.284730243
hkl_m_d_th2 0 3 1 2 1.95733178 24.3741112 I  0.2216940918
hkl_m_d_th2 1 0 2 2 1.95315433 24.4270458 I  2.875062992
hkl_m_d_th2 1 -3 1 2 1.95222831 24.4388103 I  2.043713098
hkl_m_d_th2 2 2 1 2 1.92684615 24.7658138 I  0.02774018865
hkl_m_d_th2 3 -1 -1 2 1.92162049 24.8342361 I  16.54722922
hkl_m_d_th2 3 1 -1 2 1.91873336 24.8722019 I  9.05852093
hkl_m_d_th2 1 -3 -1 2 1.91575527 24.9114876 I  0.01173116786
hkl_m_d_th2 1 -1 2 2 1.91320658 24.9452057 I  23.60225578
hkl_m_d_th2 2 -3 0 2 1.88956165 25.2624798 I  29.56832132
hkl_m_d_th2 2 0 -2 2 1.86779666 25.5618095 I  0.05974077687
hkl_m_d_th2 0 -2 2 2 1.85755312 25.7051773 I  4.36158894
hkl_m_d_th2 1 1 2 2 1.84475112 25.8866501 I  6.38744074
hkl_m_d_th2 3 -2 0 2 1.84248817 25.9189968 I  8.95762995
hkl_m_d_th2 1 3 1 2 1.83143497 26.0781727 I  9.407112421
hkl_m_d_th2 3 0 1 2 1.8312993 26.0801392 I  10.03115965
hkl_m_d_th2 2 3 0 2 1.828251 26.1243916 I  25.89582379
hkl_m_d_th2 1 2 -2 2 1.82220745 26.2125778 I  13.62178355
```

```
            hkl_m_d_th2 2 1 -2 2 1.81824589 26.27071 I  16.46117778
            hkl_m_d_th2 3 -1 1 2 1.79481769 26.6198902 I  9.352267211e-005
            hkl_m_d_th2 2 -1 -2 2 1.7857691 26.7572727 I  1.220059406
            hkl_m_d_th2 3 2 0 2 1.78551149 26.7612057 I  2.084311552
            hkl_m_d_th2 0 2 2 2 1.75479078 27.2386513 I  0.1200195344
            hkl_m_d_th2 2 3 -1 2 1.75305951 27.2660713 I  20.78355162
            hkl_m_d_th2 1 -2 2 2 1.74865687 27.3360519 I  2.077151171
            hkl_m_d_th2 3 1 1 2 1.74418604 27.4074879 I  2.388976308
            hkl_m_d_th2 1 -2 -2 2 1.74147427 27.4510002 I  8.668837292
            hkl_m_d_th2 2 -3 -1 2 1.73423302 27.5678806 I  11.94817054
            hkl_m_d_th2 3 -2 -1 2 1.72886372 27.6551952 I  0.8972588613
            hkl_m_d_th2 3 2 -1 2 1.72466445 27.723875 I  0.2418645551
            hkl_m_d_th2 2 -3 1 2 1.71871519 27.8217678 I  12.65468874
            hkl_m_d_th2 0 4 0 2 1.70948148 27.9750957 I  38.6924784
            hkl_m_d_th2 2 0 2 2 1.68763244 28.3447971 I  0.003445217182
            hkl_m_d_th2 1 -4 0 2 1.66640663 28.7135372 I  5.179661842
            hkl_m_d_th2 2 -1 2 2 1.66532505 28.7325859 I  6.513869393
            hkl_m_d_th2 2 2 -2 2 1.66415191 28.7532768 I  1.521876791
            hkl_m_d_th2 3 -2 1 2 1.65420151 28.9299927 I  10.34876388
            hkl_m_d_th2 1 2 2 2 1.6476984 29.0466785 I  0.05979760466
            hkl_m_d_th2 1 4 0 2 1.63770437 29.227869 I  2.089787806
            hkl_m_d_th2 0 -4 1 2 1.62187767 29.5195274 I  18.25260649
            hkl_m_d_th2 2 -2 -2 2 1.6152308 29.6437836 I  3.296554867
            hkl_m_d_th2 2 3 1 2 1.6141026 29.664978 I  0.8524039247
            hkl_m_d_th2 2 1 2 2 1.61287057 29.6881599 I  2.74473682
            hkl_m_d_th2 0 -3 2 2 1.60537469 29.8299904 I  26.96598698
            hkl_m_d_th2 4 0 0 2 1.60421634 29.8520298 I  3.543460163
            hkl_m_d_th2 3 0 -2 2 1.59728301 29.9846439 I  0.001599724206
            hkl_m_d_th2 3 -3 0 2 1.58763802 30.1711159 I  0.06687685381
            hkl_m_d_th2 1 3 -2 2 1.57924962 30.3352146 I  0.2402028967
            hkl_m_d_th2 3 2 1 2 1.5771724 30.3761311 I  0.3127680431
            hkl_m_d_th2 1 4 -1 2 1.5757283 30.4046421 I  0.3293136094
            hkl_m_d_th2 4 -1 0 2 1.57408154 30.4372196 I  0.3341454992
            MVW( 0.000, 187.982346`, 0.000)
            prm  s1     -0.00385 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM1+(a)strain_1(a)
            prm  s2     -0.01547 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM1+(a)strain_2(a)
            prm  s3     -0.00380 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM1+(a)strain_3(a)
```

```
            prm  s4     -0.00105 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM1+(a)strain_4(a)
            prm  s5     -0.03307 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM2+(a)strain_1(a)
            prm  s6     -0.07091 min  -0.50 max  0.50
'P2_1/m[0,0,0]GM2+(a)strain_2(a)
            prm  pe1      = +  1.00000*s1;: -0.00385
            prm  pe2      = +  1.00000*s3;: -0.00380
            prm  pe3      = +  1.00000*s4;: -0.00105
            prm  pe4      = +  1.00000*s6;: -0.07091
            prm  pe5      = +  1.00000*s2;: -0.01547
            prm  pe6      = +  1.00000*s5;: -0.03307
            straincell(6.47340,6.87020,4.28430,90.00000,95.60200,90.00000)
            celltransform(1,0,0,0,1,0,0,0,1)
                  a  = sa;:    6.44848
                  b  = sb;:    6.84409
                  c  = sc;:    4.27980
                  al = sal;:  94.06284
                  be = sbe;:  96.48413
                  ga = sga;:  91.89477
Out_file(hkl.txt)
```

Section S6. Example of an input file for program Topas 4 which was used for the parametric Le Bail fit of the strain modes for $LuF[SeO_3]$.

```
macro Out_file(file)
{
   out file append
      Out(Get(r_wp), "    \n %11.5f" ) ' _Rwp
      Out(Get(a), "%15.5f", "%9.5f") ' cell_length_a
      Out(Get(b), "%15.5f", "%9.5f") ' cell_length_b
      Out(Get(c), "%15.5f", "%9.5f") ' cell_length_c
      Out(Get(al), "%15.5f", "%9.5f") ' cell_angle_alpha
      Out(Get(be), "%15.5f", "%9.5f") ' cell_angle_beta
      Out(Get(ga), "%15.5f", "%9.5f") ' cell_angle_gamma
      Out(pe1, "%15.5f", "%9.5f")
      Out(pe2, "%15.5f", "%9.5f")
      Out(pe3, "%15.5f", "%9.5f")
      Out(pe4, "%15.5f", "%9.5f")
      Out(pe5, "%15.5f", "%9.5f")
      Out(pe6, "%15.5f", "%9.5f")
}
      '{{{macros for calculations involving the lattice parameters
      'Takes non-refinable undistorted cell parameters, and variable strains as
input.
      'Returns strained cell parameters
      macro straincell(pa0, pb0, pc0, pal0, pbe0, pga0)
      {
            prm  !radian  57.2957795
            local  palpha0 = pal0/radian;
            local  pbeta0  = pbe0/radian;
            local  pgamma0 = pga0/radian;
            'distorted parent-cell parameters
            local  pa = pa0*(pe1 + 1);:  6.44848
            local  pb = pb0*(pe2 + 1);:  6.84409
            local  pc = pc0*(pe3 + 1);:  4.27980
            local  palpha = palpha0 - pe4*Sin(palpha0);
            local  pbeta  = pbeta0  - pe5*Sin(pbeta0);
            local  pgamma = pgamma0 - pe6*Sin(pgamma0);
            local  pal = palpha*radian;: 90.07091
            local  pbe = pbeta*radian ;: 95.61740
            local  pga = pgamma*radian;: 90.03307
      }
```

```
      'Use basis-transformation matrix to transform from parent-cell to supercell
parameters
      macro celltransform(t11, t12, t13, t21, t22, t23, t31, t32, t33)
      {
            prm  !radian  57.2957795
            'parent-lattice basis vectors in cartesian coords
            local  zzz  = (Cos(palpha) - Cos(pbeta)*Cos(pgamma))/Sin(pgamma);
            local  pv11 = pa;
            local  !pv21  0
            local  !pv31  0
            local  pv12 = pb*Cos(pgamma);
            local  pv22 = pb*Sin(pgamma);
            local  !pv32  0
            local  pv13 = pc*Cos(pbeta);
            local  pv23 = pc*zzz;
            local  pv33 = pc*Sqrt(1 - Cos(pbeta)^2 - zzz^2);
            'supercell basis vectors in cartesian coords
            local  sv11 = t11*pv11 + t12*pv12 + t13*pv13;
            local  sv21 = t11*pv21 + t12*pv22 + t13*pv23;
            local  sv31 = t11*pv31 + t12*pv32 + t13*pv33;
            local  sv12 = t21*pv11 + t22*pv12 + t23*pv13;
            local  sv22 = t21*pv21 + t22*pv22 + t23*pv23;
            local  sv32 = t21*pv31 + t22*pv32 + t23*pv33;
            local  sv13 = t31*pv11 + t32*pv12 + t33*pv13;
            local  sv23 = t31*pv21 + t32*pv22 + t33*pv23;
            local  sv33 = t31*pv31 + t32*pv32 + t33*pv33;
            'distorted supercell parameters
            local  sa = Sqrt(sv11^2+sv21^2+sv31^2);
            local  sb = Sqrt(sv12^2+sv22^2+sv32^2);
            local  sc = Sqrt(sv13^2+sv23^2+sv33^2);
            local  salpha = ArcCos((sv12*sv13+sv22*sv23+sv32*sv33)/(sb*sc));
            local  sbeta  = ArcCos((sv11*sv13+sv21*sv23+sv31*sv33)/(sa*sc));
            local  sgamma = ArcCos((sv11*sv12+sv21*sv22+sv31*sv32)/(sa*sb));
            local  sal = salpha*radian;
            local  sbe = sbeta*radian;
            local  sga = sgamma*radian;
      }
 '}}}
bootstrap_errors 100
approximate_A
```

```
prm !t_kr 120

prm pA_e1  0.049`
prm pB_e1  757.51398`
prm pA_e2  0.02951`
prm pB_e2  750.70520`
prm pA_e3  0.00188`
prm pB_e3  1611.79064`
prm pA_e4  0.68113`
prm pB_e4  113.43002`
prm pA_e5  0.90131`
prm pB_e5  317.62995`
prm pA_e6  0.94034`
prm pB_e6  221.29718`
prm up_beta  0.40009`

macro parametric {
      local Tdiff = (t_kr - t_cur) / t_kr;
      local ppA_e1 = pA_e1 * 0.00001;
      local ppA_e2 = pA_e2 * 0.00001;
      local ppA_e3 = pA_e3 * 0.00001;
      local ppA_e4 = pA_e4 * 0.001;
      local ppA_e5 = pA_e5 * 0.00001;
      local ppA_e6 = pA_e6 * 0.0001;

      local  s1 =  0.000052109 + t_cur * 0.00000733868 - ((ppA_e1*Tdiff)^(up_beta))
* (1- (2/ (Exp(2*Tdiff*pB_e1* ((ppA_e1*Tdiff)^(up_beta)) )+1 ) ) ) ;
      local  s3 = -0.000470013 + t_cur * 0.00000495331 - ((ppA_e2*Tdiff)^(up_beta))
* (1- (2/ (Exp(2*Tdiff*pB_e2* ((ppA_e2*Tdiff)^(up_beta)) )+1 ) ) ) ;
      local  s4 = -0.000280688 + t_cur * 0.00000131401 - ((ppA_e3*Tdiff)^(up_beta))
* (1- (2/ (Exp(2*Tdiff*pB_e3* ((ppA_e3*Tdiff)^(up_beta)) )+1 ) ) ) ;
      local  s6 = 0 - ((ppA_e4*Tdiff)^(up_beta)) * (1- (2/ (Exp(2*Tdiff*pB_e4*
((ppA_e4*Tdiff)^(up_beta)) )+1 ) ) ) ;
      local  s2 = -0.00239     + t_cur * 0.0000240263  - ((ppA_e5*Tdiff)^(up_beta))
* (1- (2/ (Exp(2*Tdiff*pB_e5* ((ppA_e5*Tdiff)^(up_beta)) )+1 ) ) ) ;
      local  s5 = 0 - ((ppA_e6*Tdiff)^(up_beta)) * (1- (2/ (Exp(2*Tdiff*pB_e6*
((ppA_e6*Tdiff)^(up_beta)) )+1 ) ) ) ;

      local  pe1      = +  1.00000*s1;: -0.00385
      local  pe2      = +  1.00000*s3;: -0.00380
      local  pe3      = +  1.00000*s4;: -0.00105
```

```
      local  pe4      = +  1.00000*s6;: -0.07091
      local  pe5      = +  1.00000*s2;: -0.01547
      local  pe6      = +  1.00000*s5;: -0.03307
      straincell(6.47340,6.87020,4.28430,90.00000,95.60200,90.00000)
      celltransform(1,0,0,0,1,0,0,0,1)
      a  = sa;
      b  = sb;
      c  = sc;
      al = sal;
      be = sbe;
      ga = sga;
}
do_errors
XYE(FileName)
      bkg @  11709.2632` -7270.52638`  1807.12667`  559.698689` -327.151394`
59.2198455` -27.9445084`  134.076664`  129.903703`  104.599382` -82.3954619`
      start_X  4
      LP_Factor( 90)
      Zero_Error(, -0.0138)
      convolution_step 5
      Rp 217.5
      Rs 217.5
      Simple_Axial_Model( 0.001)
      lam
            ymin_on_ymax  0.0001
            la  1 lo  0.826401 lh  0.0001
      x_calculation_step 0.001

      local !t_cur 26.4

      hkl_Is
            lebail  1
            LVol_FWHM_CS_G_L( 1, 371.73081`, 0.89, 358.97949`,@,
412.35940`_LIMIT_MIN_0.3,@, 10000.00000`_LIMIT_MIN_0.3)
            e0_from_Strain( 0.04225`,lg32, 0.16898`,lg32, 0.16898`)
            r_bragg  0.391664467
            phase_name "hkl_P-1"
            space_group "P-1"
            load hkl_m_d_th2 I
            {
                  0   1   0   2    6.83805        6.92861  0.024746976
```

1	0	0	2	6.41715	7.38367	3.91833743
1	-1	0	2	4.76305	9.95348	1.95279846
1	1	0	2	4.59989	10.30747	2.19829103
0	0	1	2	4.24747	11.16532	35.4301596
1	0	-1	2	3.73571	12.70076	15.0139436
0	-1	1	2	3.71500	12.77186	0.514215051
0	1	1	2	3.50987	13.52167	0.301598166
0	2	0	2	3.41902	13.88271	41.7200628
1	0	1	2	3.37541	14.06300	0.00965341159
1	1	-1	2	3.32825	14.26329	0.015741823
1	-1	-1	2	3.23069	14.69633	0.0622192814
2	0	0	2	3.20857	14.79821	0.783841376
1	-1	1	2	3.11276	15.25639	6.2565887
1	-2	0	2	3.06215	15.51007	3.94958044
1	2	0	2	2.97467	15.96912	0.262972008
1	1	1	2	2.94748	16.11742	0.682246278
2	-1	0	2	2.94450	16.13383	35.3165712
2	1	0	2	2.86647	16.57605	21.2494837
0	-2	1	2	2.74972	17.28512	11.0410951
2	0	-1	2	2.70715	17.55908	0.287663831
0	2	1	2	2.58465	18.39836	5.03708848
1	2	-1	2	2.56776	18.52045	4.52744489
2	1	-1	2	2.52650	18.82560	10.5987918
2	-1	-1	2	2.50775	18.96768	8.29112031
1	-2	1	2	2.48901	19.11184	0.714758468
1	-2	-1	2	2.47890	19.19052	8.70722257
2	0	1	2	2.43484	19.54117	0.0045915165
2	-2	0	2	2.38152	19.98307	0.115084831
2	-1	1	2	2.34067	20.33554	15.3077497
1	2	1	2	2.32361	20.48646	0.203657649
2	2	0	2	2.29994	20.69953	0.654754332
0	3	0	2	2.27935	20.88865	2.14257628
2	1	1	2	2.24957	21.16830	3.8556419
1	-3	0	2	2.17193	21.93427	5.47330838
3	0	0	2	2.13905	22.27571	13.4310804
2	2	-1	2	2.13374	22.33188	1.59925821
1	3	0	2	2.12461	22.42902	2.29348514
0	0	2	2	2.12373	22.43843	17.0513902
2	-2	-1	2	2.11125	22.57285	5.01758677
1	0	-2	2	2.08566	22.85355	10.8027288
0	-1	2	2	2.06554	23.07919	0.0270627272

0	-3	1	2	2.06358	23.10133	0.546757305
3	-1	0	2	2.06211	23.11806	4.94936706
2	-2	1	2	2.04490	23.31537	3.63708017
1	1	-2	2	2.02383	23.56159	0.246170742
3	1	0	2	2.02149	23.58926	7.08766494
3	0	-1	2	2.00075	23.83729	2.21456699
0	1	2	2	1.99276	23.93434	0.0381457235
1	3	-1	2	1.97707	24.12703	0.884439619
1	-1	-2	2	1.96723	24.24963	1.59091136
0	3	1	2	1.95747	24.37234	0.290096333
1	0	2	2	1.95323	24.42607	1.49976884
1	-3	1	2	1.95218	24.43945	3.7225812
2	2	1	2	1.92698	24.76405	0.0357697151
3	-1	-1	2	1.92172	24.83298	15.3702146
3	1	-1	2	1.91878	24.87165	10.5021546
1	-3	-1	2	1.91588	24.90979	0.000554760994
1	-1	2	2	1.91322	24.94506	23.8592822
2	-3	0	2	1.88960	25.26190	29.9266132
2	0	-2	2	1.86786	25.56098	0.0611182032
0	-2	2	2	1.85750	25.70593	4.5347546
1	1	2	2	1.84487	25.88488	6.23538139
3	-2	0	2	1.84255	25.91813	9.53611491
1	3	1	2	1.83156	26.07629	10.3017915
3	0	1	2	1.83138	26.07892	6.34041753
2	3	0	2	1.82831	26.12359	29.0195537
1	2	-2	2	1.82216	26.21331	14.5588336
2	1	-2	2	1.81825	26.27061	15.8913536
3	-1	1	2	1.79487	26.61911	6.28905689e-006
2	-1	-2	2	1.78587	26.75572	1.35247204
3	2	0	2	1.78558	26.76012	1.94795434
0	2	2	2	1.75494	27.23635	0.00078025157
2	3	-1	2	1.75304	27.26639	21.2171818
1	-2	2	2	1.74862	27.33659	1.66479242
3	1	1	2	1.74429	27.40586	1.67610647
1	-2	-2	2	1.74161	27.44878	9.36480741
2	-3	-1	2	1.73434	27.56618	11.9615474
3	-2	-1	2	1.72896	27.65365	1.35138474
3	2	-1	2	1.72468	27.72359	0.239750293
2	-3	1	2	1.71870	27.82206	12.735513
0	4	0	2	1.70951	27.97458	39.181141
2	0	2	2	1.68770	28.34357	0.00092284731

```
                    1  -4   0   2    1.66644       28.71302  4.26644262
                    2  -1   2   2    1.66535       28.73210  8.31600931
                    2   2  -2   2    1.66412       28.75377  0.716769313
                    3  -2   1   2    1.65422       28.92959  10.6894532
                    1   2   2   2    1.64783       29.04427  0.0229028229
                    1   4   0   2    1.63774       29.22722  2.86629758
                    0  -4   1   2    1.62184       29.52029  18.6687268
                    2  -2  -2   2    1.61535       29.64162  3.37294527
                    2   3   1   2    1.61421       29.66295  0.617988899
                    2   1   2   2    1.61297       29.68622  2.88230491
                    0  -3   2   2    1.60531       29.83119  29.1986885
                    4   0   0   2    1.60429       29.85070  1.49953387
                    3   0  -2   2    1.59734       29.98363  0.000422094507
                    3  -3   0   2    1.58768       30.17026  0.0319418927
                    1   3  -2   2    1.57919       30.33638  0.163447899
                    3   2   1   2    1.57727       30.37417  0.210912489
                    1   4  -1   2    1.57570       30.40529  0.235003204
                    4  -1   0   2    1.57415       30.43595  0.26096073
            }
            MVW( 0.000, 188.005031`, 0.000)
parametric

Out_file(hkl_param.txt)
```