Electronic Supplementary Material (ESI) for Dalton Transactions


# Supporting material:
# Combined x-ray and neutron diffraction study of vacancies and disorder dimorphic clathrate$Ba_8Ga_{16}Sn_{30}$ of type I and VIII

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## Hamilton tests:

Hamilton tests are a useful tool to determine if one model gives a better description than another, taking into account difference in the number of parameters for each model.[1] The test is based on the factor $R_h$, which is the ratio between $R_w$ values for each model, and the statistical factor R calculated from the number of model-parameters and the number of observed reflections. $R_h > R$ demonstrates that anharmonic atomic displacement parameters (ADP) offers a significantly better description of the data. For 1BGS the anharmonic ADPs clearly improves the model at all temperatures for both x-ray and neutron data. For n-8BGS the anharmonic model offers a better description of neutron data at low temperature (10 K - 100K) and at high temperature (400 K, 500 K). For p-8BGS the anharmonic ADPs only improve the model at 200 K and 300 K. At all temperature is the description of x-ray data improved by the anharmonic model. The difference between $R$ and $R_h$ is greater for the x-ray because of the better data quality. From looking at the scales of Figure 1 it is clear at that anharmonic effects and static disorder described by the anharmonic model are much more expressed in 1BGS compared to 8BGS.

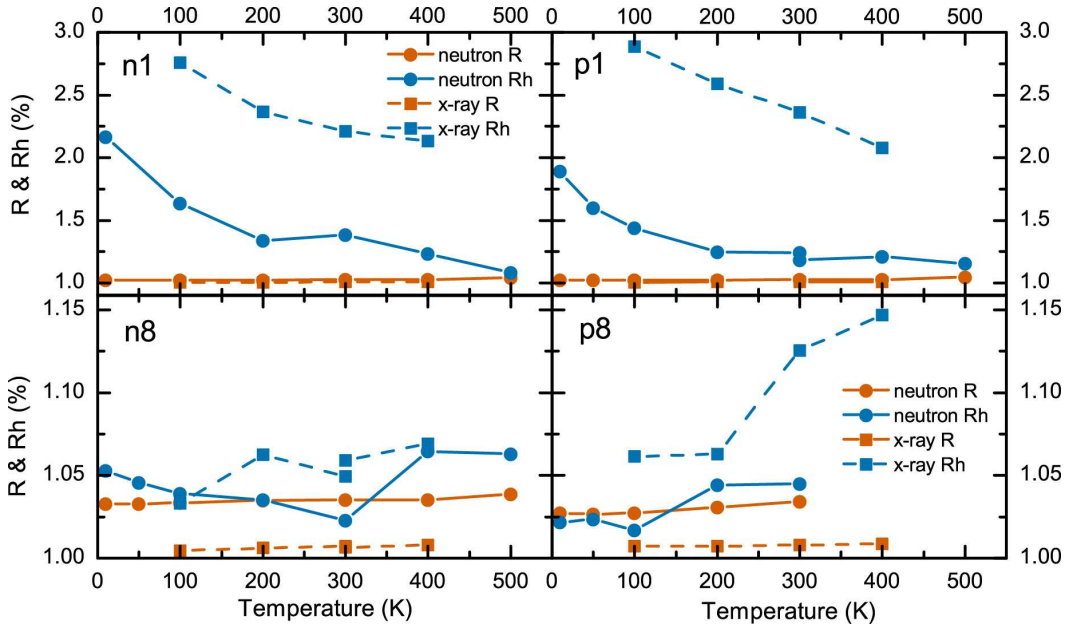

**Figure 1 Hamilton tests for comparison of models with anisotropic and anharmonic description of the guest atoms on 6d (1BGS) and 8c (8BGS) sites. $R_h$ > R entail that the anharmonic model (with more parameters) offers at significantly better description of the data compared to the anisotropic model.**

## Occupancies:

The occupancy of Sn is plotted for all framework sites in Figure 2 (1BGS) and Figure 3 (8BGS). Occupancies were restricted so that the fractional occupation of Ga was: $occ_{Ga} = 1 - occ_{Sn}$. In 1BGS the 6*c* site shows the highest affinity for Ga (typical for type I clathrates), while it in 8BGS is the 8*c* site.

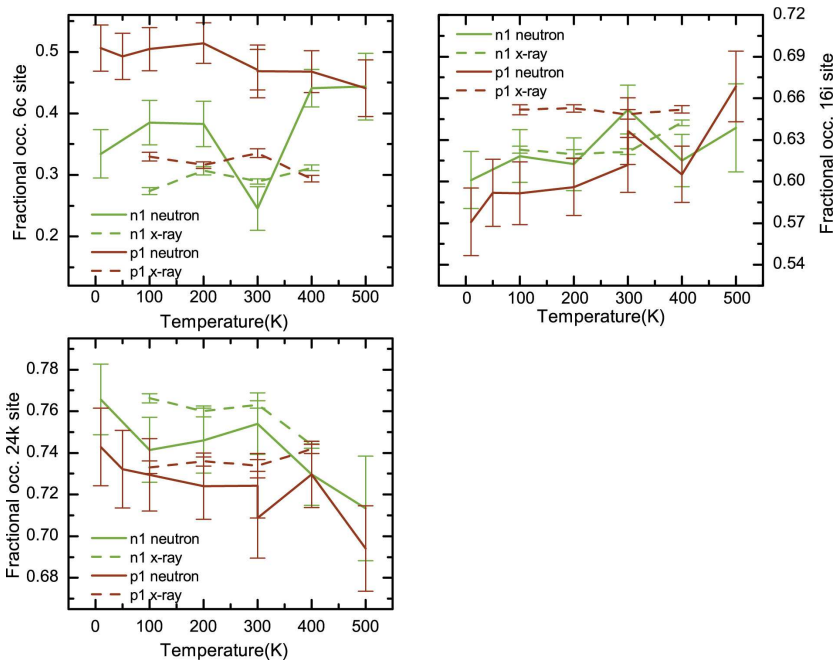


**Figure 2 Fractional occupancy of Sn on all framework positions in 1BGS**

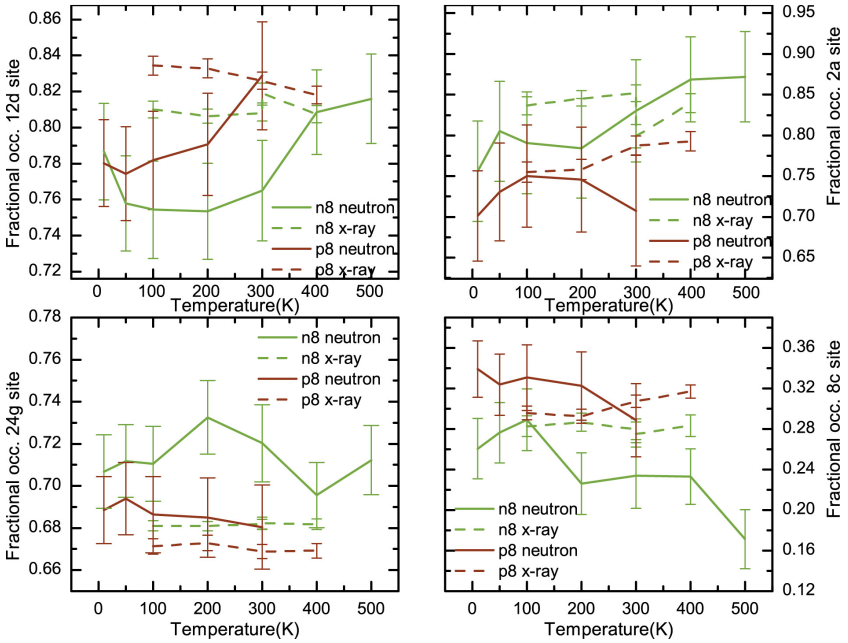


Figure 3 Fractional occupancy of Sn on all framework positions in 8BGS

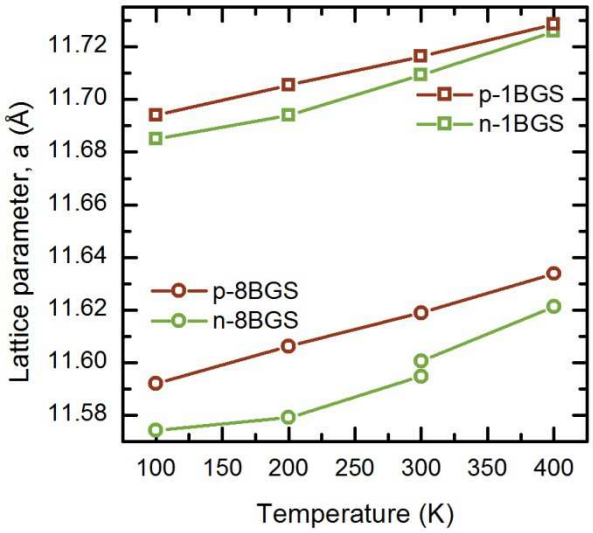


Figure 4 Lattice parameters of 1BGS (squares) and 8BGS (circles) determined by single crystal x-ray diffraction

## Refinement of anharmonic thermal parameters:

Probability distribution functions of guest atoms at all temperatures:

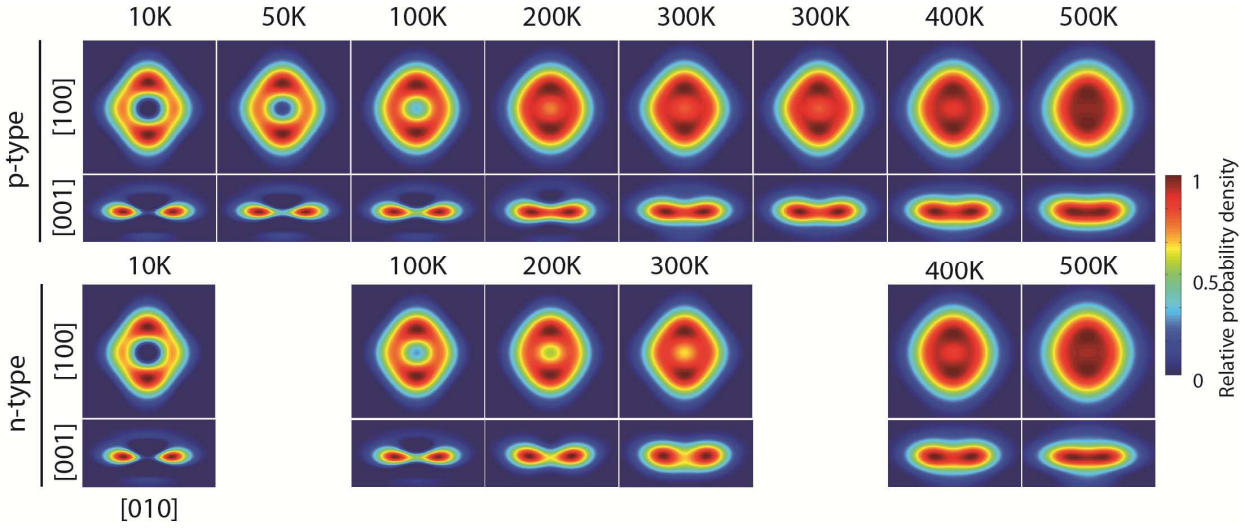


**Figure 5 Comparison of probability distribution functions for n- and p-type 1BGS. No difference between n- and p-type can be observed.**

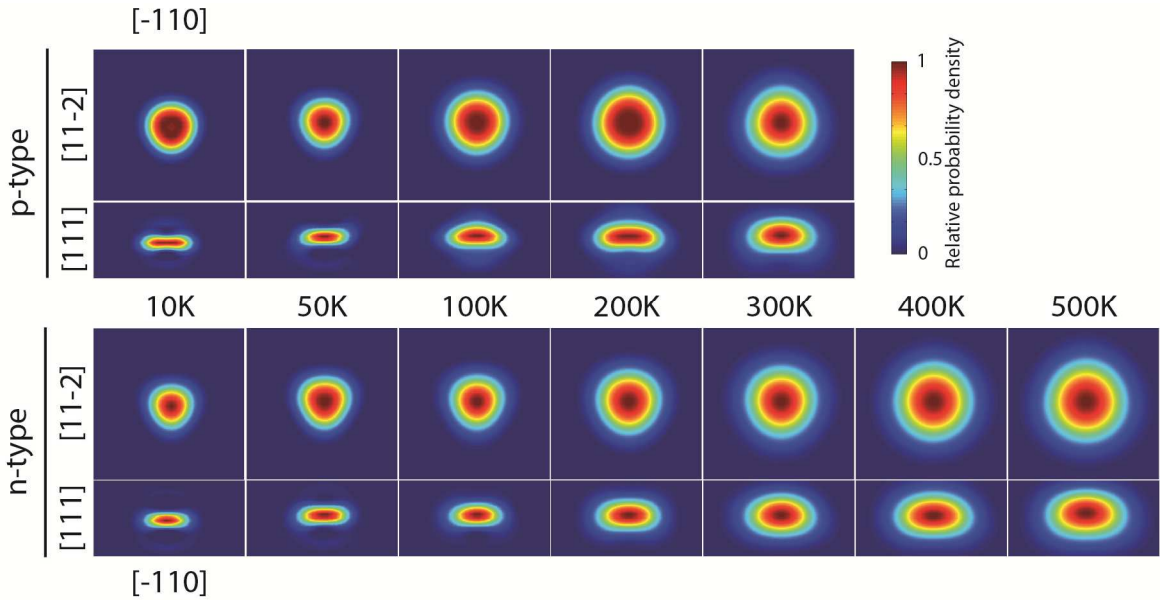


**Figure 6 Comparison of probability distribution functions for n- and p-type 8BGS. No difference between n- and p-type can be observed.**

## Maximum Entropy Method (MEM):

The convergence criteria for MEM calculations is determined by the procedure described in [1]. The procedure dictates that the optimal MEM solution is the one showing the most Gaussian distribution of residual density, $\rho_{res.}$ calculated by the inverse Fourier transform of the difference, $F_{obs}(\boldsymbol{H}) - F_{MEM}(\boldsymbol{H})$. This is evaluated from the fractal dimension plot which is the logarithm of the residual density histogram. The fractal dimension plot of a perfect Gaussian distribution is a parabola, so the most Gaussian distribution is quantified, by fitting the fractal dimension with a function of the form: $f(x) = c_1x^2 + c_2$.

Figure 7 shows fractal dimension plots for MEM calculations on n-1BGS (T=100 K) for various stopping criteria and both uniform (left) and nonuniform prior densities (middle & right). It is clear that to achieve convergence it is essential to use a non-uniform prior density based on knowledge of the structure. In our

case we used 3 types of non-uniform priors. The experimental thermal parameters were used for all framework atoms and Ba(1) (for 1BGS). Thermal parameters of Ba(2) (1BGS) and Ba(1) (8BGS) were fixed and severely underestimated ("*Localized guest atom*"-prior) or severely overestimated ("*Smeared guest atom*"-prior). This was done to avoid model bias in the guest atom description.The third prior was based on the "24k-model" where the guest atom was displaced from the 6*d* to the 24*k* site. For x-ray data we obtained approximately Gaussian residual density distributions for $\chi^2_{aim} = 0.7 - 1.5$, Figure 7. Plots of the electron density around the Ba(2) guest atom does not show major changes dependant on $\chi^2_{aim}$ in this range, Figure 9. For MEM calculations based on Laue neutron data the choice of prior did somewhat affect the fractal dimension plot. However; none of the stopping criteria gave Gaussian distributions of the residual density, Figure 8. Furthermore; for 1BGS the fractal dimension plots most resembling parabolas exhibited unphysical features in the nuclear distribution, Figure 11. So far it appear to be more difficult to determine optimal convergence criteria for MEM calculations based on Laue data compared to x-ray data.

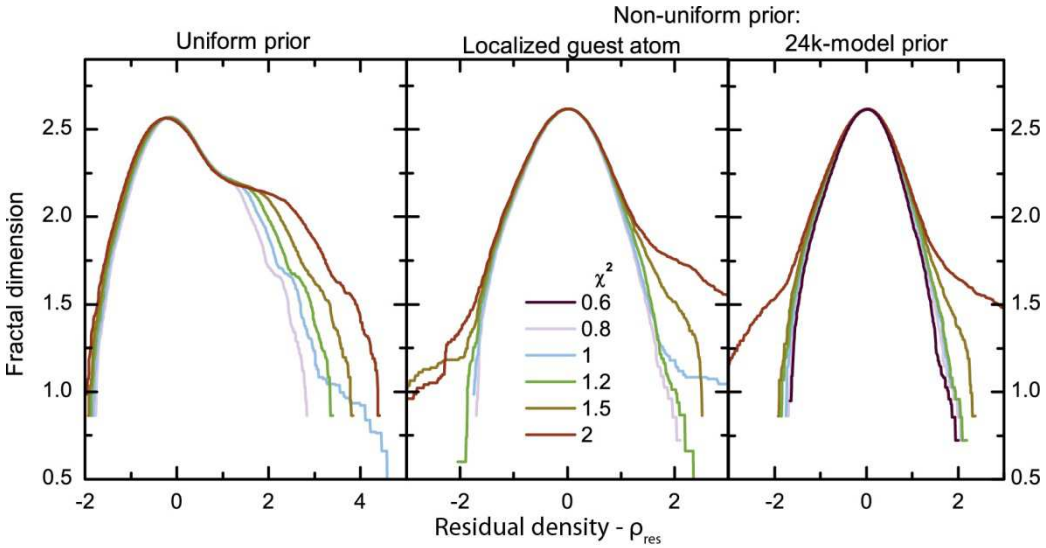


**Figure 7 Fractal dimension plots for MEM solutions for n-1BGS using various stopping criteria based on x-ray data. The optimal MEM solution has a parabolic fractal dimension plot. Application of a procrystal prior density (middle & right) is essential to reach the optimum. MEM solutions based started from a flat prior (left) will have a highly asymmetric residual distribution and not reach an optimal solution.**

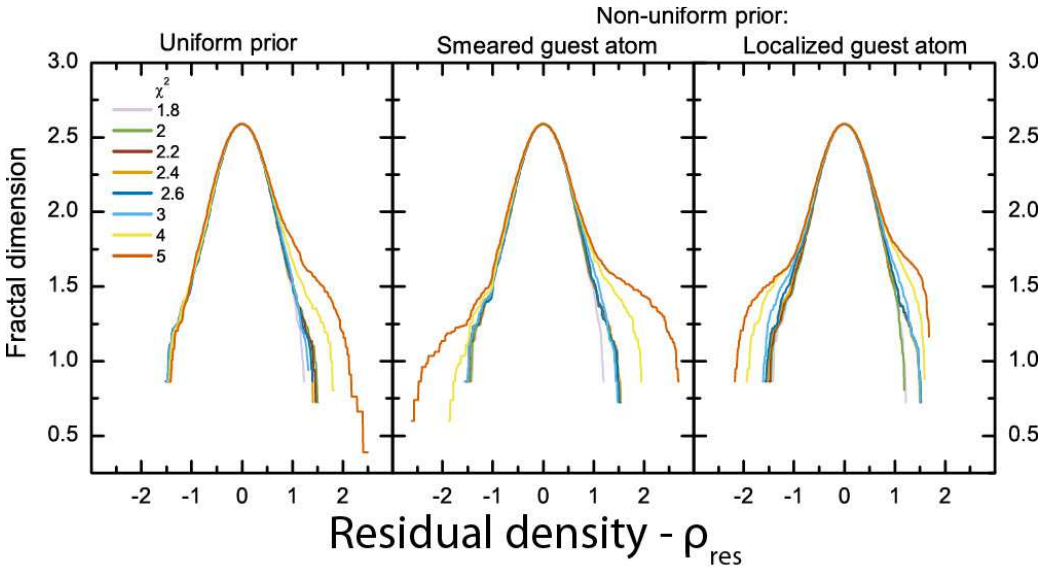


**Figure 8 Fractal dimension plot for MEM solutions for n-1BGS based on neutron Laue data for different choices of prior density. (left) Flat uniform prior, (middle, right) Procrystal prior density based on refined structure. The thermal parameters of the guest atom were increased (middle) and strongly decreased (right) to reduce bias toward the refined structure.**

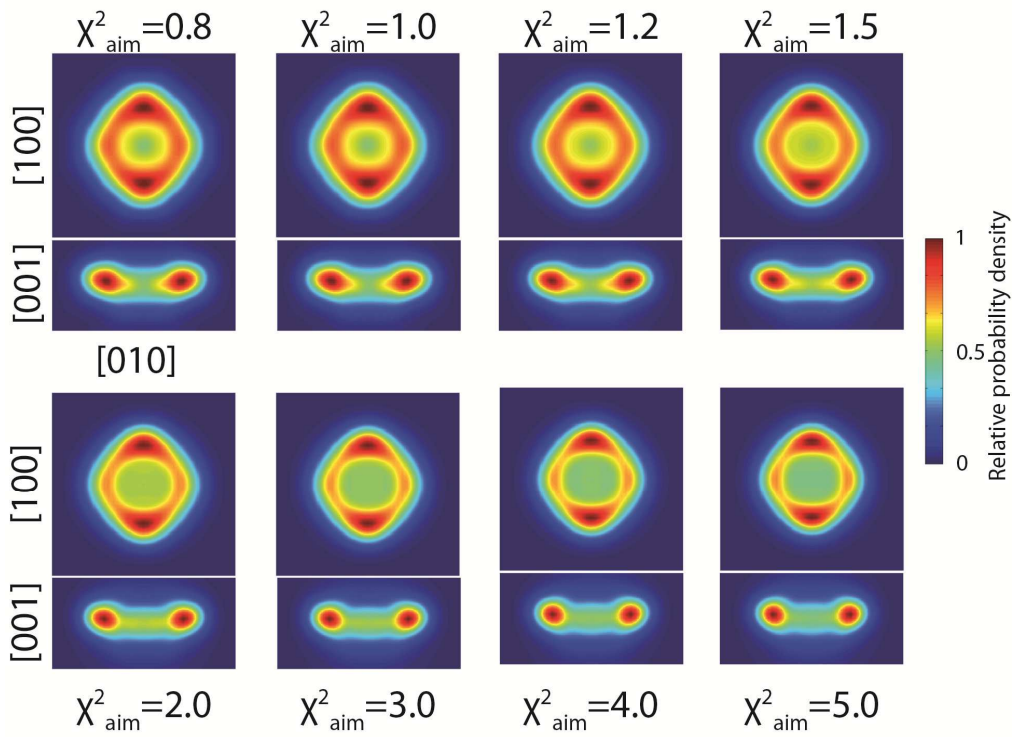


**Figure 9: Electron distribution from MEM-calculations based on X-ray data on n1BGS at T=100K using different stopping criteria. The choice of stopping criteria does not affect the major features around the Ba(2) guest atom near the 6*d* site. The dimensions of the plots are 2.4 Å x 2.4 Å.**

The electron distribution around the 6*d* site determined by MEM is qualitatively independent of the stopping criteria, Figure 9.

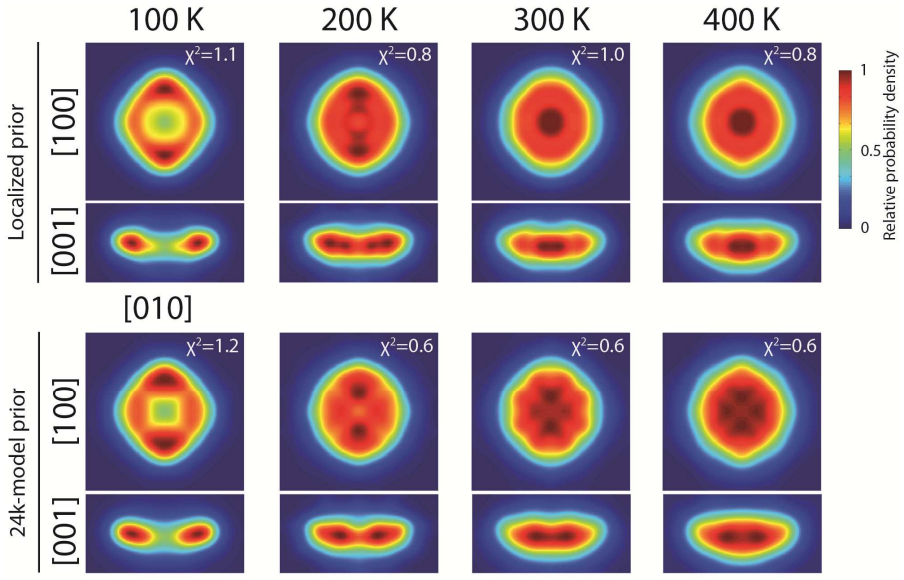


**Figure 10 Electron density from MEM calculations on n-1BGS for 2 different prior densities. (top) in the prior density the Ba guest atoms was located on the 6d-site and (bottom) on the 24k site. Atomic position obtained from refinement of "24k-model" . $\chi^2$-stopping criteria chosen based on parabolic fit to fractal dimension.**

Dynamic electron densities of n-1BGS using optimized stopping criteria at various temperatures are shown in, Figure 10. Above 100 K thermal smearing causes the MEM electron density to depend heavily on the choice of prior. Only the "24k-model prior" gives a maximum in electron density correctly displaced from the 6*d* site. For neutron data the obtained MEM density is much less affected by the choice of prior and it is thus better suited for studying disorder; especially at elevated temperatures.

Figure 11 shows dynamic nuclear distributions obtained from neutron Laue data at 100K on n1BGS at various stopping criteria. For stopping criteria lower than $\chi^2_{aim} = 4$, unphysical features close to the guest atom positions start to appear. A stopping criterion of 4 corresponds to a residual density distribution which is asymmetric and far from Gaussian, Figure 8.

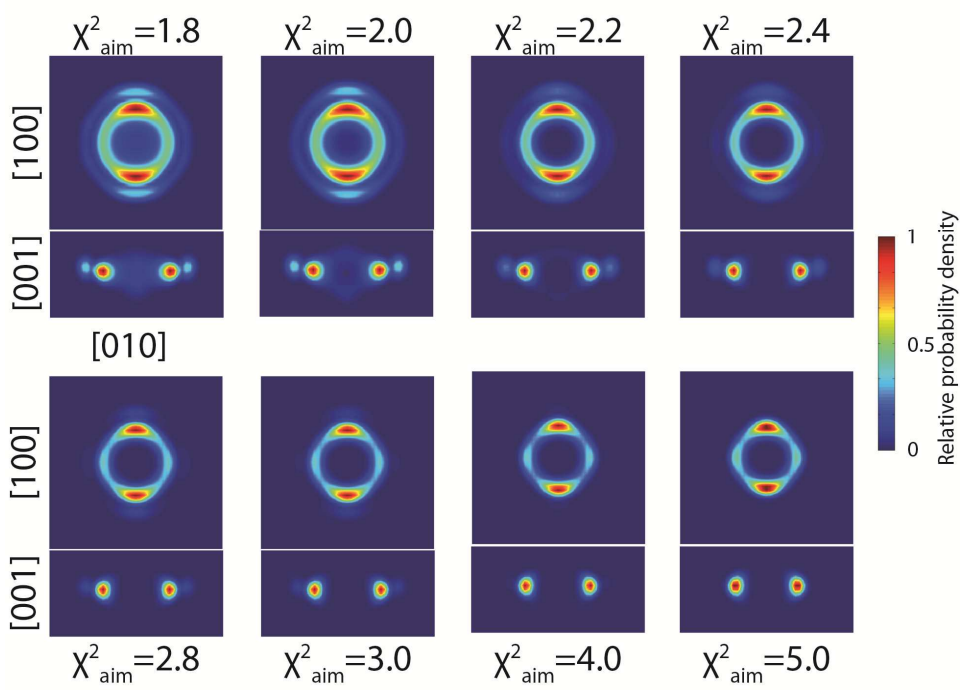


**Figure 11 Nuclear density distribution of obtained from neutron Laue data at 100K on n1BGS obtained for different stopping criteria for the MEM calculations. The dimensions of the plots are 2.4 Å x 2.4 Å.**

For neutron data on 8BGS the qualitative nuclear distribution of the guest atom is not affected by the choice of stopping criteria, as shown in Figure 12. We are therefore confident that the choice of stopping criteria does not affect out conclusion that no guest atom disorder is present in 8BGS.

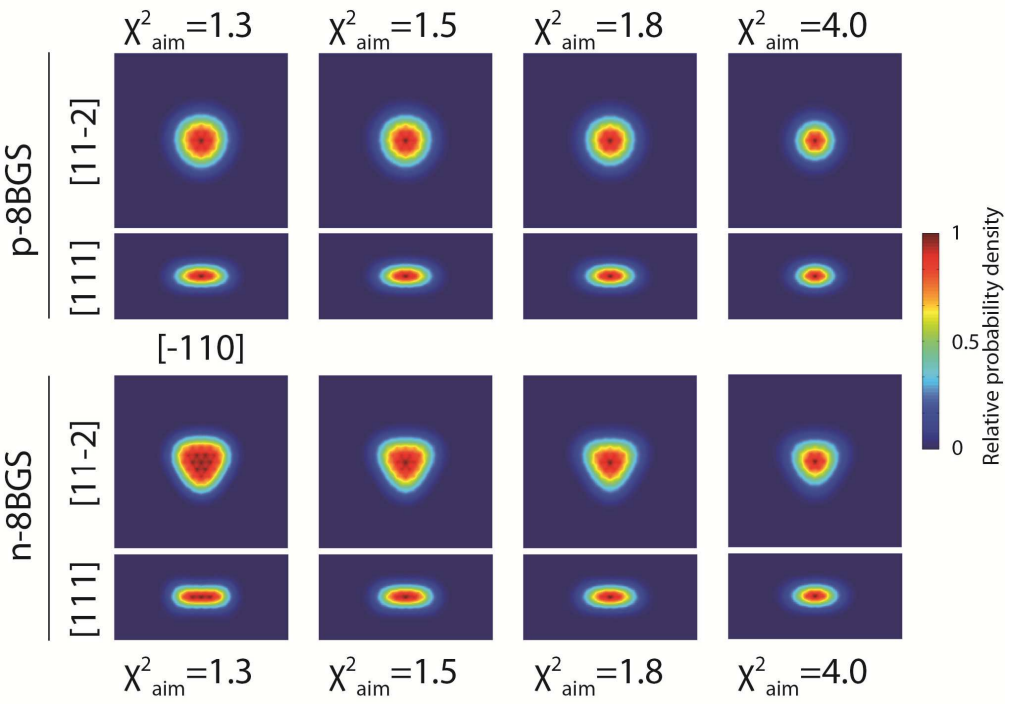


**Figure 12 Nuclear density distribution of p- and n-8BGS determined by the MEM using various stopping criteria. Calculations are based on neutron Laue data collected at 10 K. The qualitative features of the MEM density is not affected by the choice of stopping criteria. The dimensions of the plots are 1.6 Å x 1.6 Å.**

In the present case of MEM based on Laue diffraction data there is significant problems of determining the stopping criteria for the optimal MEM solution. The choice of stopping criteria seriously affects the final MEM density; hence there is a serious danger of over fitting the data. It should be further investigated why Laue data appear to be ill-suited for the MEM. Reasons for the convergence problems which should be investigated are: 1) The missing high intensity reflections which is intrinsic to the Laue technique will cause severe Gibbs oscillations in the residual density, $\rho_{res}$ used for evaluation of convergence. 2) The MEM relies heavily on standard errors of the observed intensities; hence incorrect evaluation these during the data integration and merging procedure could adversely affect the MEM solution.

## Atomic displacement parameters:

The harmonic thermal displacement parameters (*U*) was modelled using Einstein model [2] for guest atoms and the Debye model for the framework atom.[3]

**Type I: Both guest atoms Ba(1) (2*a*) and Ba(2) (24*k*) were modelled isotropically in the "24*k*"-model, Figure 13 (left) for n1BGS (no significant difference is observed between n- and p-type).**

Table 1 gives the Einstein temperature, $T_E$ and disorder parameter, *d* extracted from fits to *U*. Values are identical for n- and p-type within uncertainties. As expected the Einstein temperature is substantially lower for Ba(2) compared to Ba(1), and for both guest atoms $T_E$ is in good agreement with values determined for other type I clathrates.[4] Framework atoms were modelled anisotropically thus average ADPs are plotted, Figure 13 (bottom left). For fitting of the Debye model we calculated the average mass of each lattice site, Table 2, from joint neutron and x-ray refinement occupancies. All lattice sites had very similar *U* and the extracted Debye-temperatures, $T_D$ of 176-198K is in the expected range considering the mass of framework

atoms. Results are in agreement with previous reports for 1BGS[5]. The values are intermediate between those obtained for $Ba_8Ga_{16}Ge_{30}$[6, 7] and $A_8Sn_{44}\square_2$ (A=Rb, Cs, □=vacancy).[8]

**Type VIII: The guest atom was modelled anisotropically, thus maximal (perpendicular to [111]), minimal (parallel to [111]) and average displacements *U* are given, Figure 13(top right) for n-8BGS. The Einstein temperature, $T_E$=59(1) (n-8BGS), 56(1)K (p-8BGS),**

Table 1 for movement orthogonal to [111] is significantly decreased compared to Ba(2) in 1BGS, thus the rattler energy of 8BGS is expected to be slightly lower. Average U's are comparable to type I.

The framework ADPs are not as uniform for 8BGS compared to 1BGS. The difference can be attributed to larger spread in bond lengths and angles for various framework sites. The disorder parameter, *d* is significantly increased for the 12*d* framework site compared to all other framework sites. This indicates that the atom could be more accurately described using a split-site model; however this is not the aim of the present study. The result are in reasonable agreement with previous results on 8BGS where a common Debye temperature of $T_D = 195\ K$ was determined for all framework atoms.[9]

The difference in Debye temperature between n- and p-type 1BGS and 8BGS is not considered significant considering standard deviations and the spread in reported Debye temperatures for related compounds.[4]

ADPs determined by x-ray and neutron diffraction are compared in Figure 14. ADPs from x-ray data are systematically slightly lower compared to values determined from neutron data.

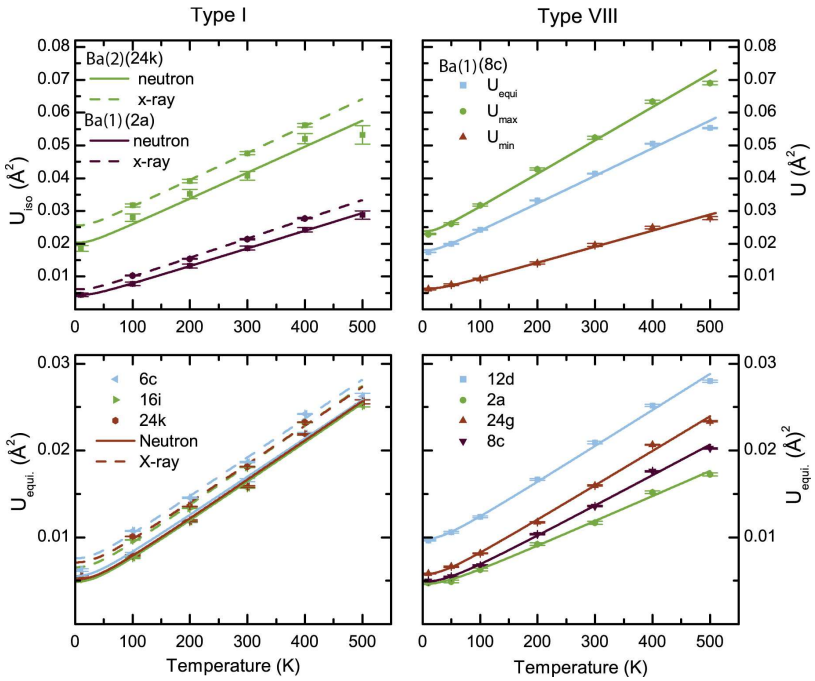


**Figure 13 Atomic displacement parameters of guest atoms (top) and framework atoms (bottom) in n1BGS (left) and n8BGS (right). No significant difference was observed between n- and p-type in either case, thus p-type data has been omitted.**

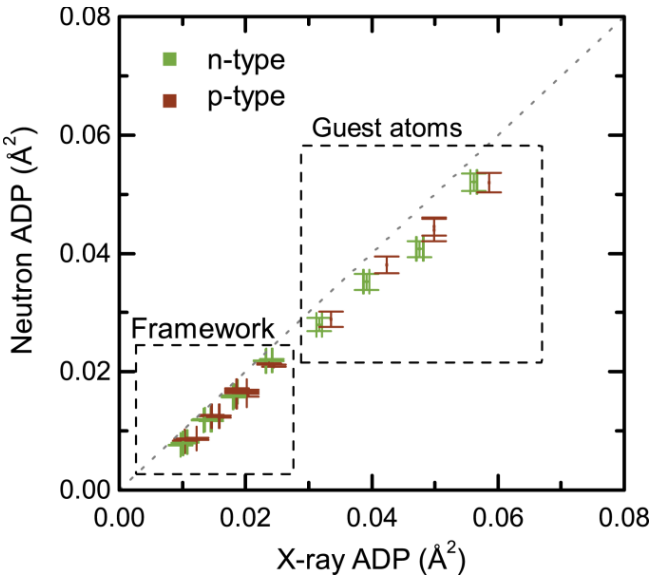


**Figure 14 Comparison of ADPs obtained separately from the neutron and x-ray data from n-1BGS (green) and p-1BGS (red). The dotted grey line indicates equal ADPs.**

**Table 1 Einstein temperatures, $T_E$ and disorder parameters d determined refinement of neutron data with *24k-model* for type I and anisotropic model for type VIII.**

| | 1BGS | | | | 8BGS | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | $T_{E,Ba(1)}$/K | $d_{Ba(1)}$/K | $T_{E,Ba(2)}$/K | $d_{Ba(2)}$/Å | $T_{E,eq}$/K | d/Å | $T_{E,max}$/K | d/Å | $T_{E,min}$/K | d/Å |
| n-type | 80.8(8) | 0.048(3) | 67(4) | 0.133(9) | 64(1) | 0.123(3) | 59(1) | 0.145(4) | 85(2) | 0.065(4) |
| p-type | 86(3) | 0.056(7) | 66(3) | 0.137(7) | 62(1) | 0.118(3) | 56(1) | 0.139(3) | 80(2) | 0.055(4) |

**Table 2 Debye temperature for host structure atoms determined from neutron diffraction. Anharmonic thermal parameters were used to describe the guest atom movement.**

| 1BGS | n-type | | | p-type | | |
|---|---|---|---|---|---|---|
| | $T_D$/K | d/Å | $m_{av.}$/au | $T_D$/K | d/Å | $m_{av.}$/au |
| 6c | 194(4) | 0.061(4) | 87.2 | 199(3) | 0.067(2) | 92.4 |
| 16i | 182(4) | 0.056(5) | 98.9 | 190(5) | 0.064(3) | 98.3 |
| 24k | 177(4) | 0.058(4) | 104.6 | 184(2) | 0.066(2) | 103.7 |

| 8BGS | n-type | | | p-type | | |
|---|---|---|---|---|---|---|
| | $T_D$/K | d/Å | $m_{av.}$/au | $T_D$/K | d/Å | $m_{av.}$/au |
| 12d | 181(3) | 0.089(2) | 106.6 | 178(3) | 0.086(1) | 107.2 |
| 2a | 216(3) | 0.055(2) | 107.6 | 205(7) | 0.054(3) | 103.2 |
| 24g | 188(3) | 0.062(2) | 103.0 | 183(4) | 0.060(2) | 101.9 |
| 8c | 225(2) | 0.054(2) | 81.2 | 214(4) | 0.052(2) | 84.9 |

## References


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[5] Suekuni K, Avila M A, Umeo K, Fukuoka H, Yamanaka S, Nakagawa T and Takabatake T 2008 *Phys. Rev. B* **77** 235119

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[7] Sales B C, Chakoumakos B C, Jin R, Thompson J R and Mandrus D 2001 *Phys. Rev. B* **63** 245113

[8] Kaltzoglou A, Fassler T, Christensen M, Johnsen S, Iversen B, Presniakov I, Sobolev A and Shevelkov A 2008 *J. Mater. Chem.* **18** 5630-7

[9] Huo D, et al. 2005 *Phys. Rev. B* **71** 075113

## Refined parameters: 1BGS

Refined parameters for all refinements of all models used in the paper are reported below. Occupancies are given as calculated by JANA2006:

$ai = (fractional\ occupancy) \cdot (site\ multiplicity)\ /\ (number\ of\ symmetry\ operators)$.

**Table 3 Crystallographic details and refined parameters from refinement of "Anharmonic"-model against x-ray data of n-1BGS**

| n-1BGS "*Anharmonic model*" | | Radiation source: | | | X-ray |
|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 400 |
| $N_{par}$ | | 23 | 23 | 23 | 23 |
| $N_{obs}$ | | 1545 | 1564 | 1559 | 1583 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 1221 | 1136 | 1014 | 922 |
| $R_F$ | | 3.60 | 3.80 | 4.45 | 5.19 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 2.45 | 2.22 | 2.07 | 2.18 |
| $R_{wF}$ | | 3.30 | 3.97 | 2.81 | 2.85 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 3.14 | 2.64 | 2.50 | 2.44 |
| $R_{internal}$ | | 2.74 | 2.86 | 2.94 | 3.11 |
| extinction | | 0.051(7) | 0.054(8) | 0.059(5) | 0.089(6) |
| Ba(1) 2a | $U_{11}$ | 0.01024(9) | 0.0155(1) | 0.0213(1) | 0.0276(1) |
| Ba(2) 6d | $U_{11}$ | 0.0190(5) | 0.0266(8) | 0.0344(6) | 0.0431(7) |
| | $U_{22}$ | 0.1281(6) | 0.1320(9) | 0.1421(7) | 0.1539(8) |
| | $C_{122}$ | 0.0066(2) | 0.0056(2) | 0.0052(2) | 0.0057(2) |
| | $D_{1111}$ | 0.00005(5) | 0.00008(8) | 0.00004(7) | 0.00006(10) |
| | $D_{1122}$ | -0.00008(5) | -0.00015(7) | -0.00025(6) | -0.00040(7) |
| | $D_{2222}$ | -0.0184(3) | -0.0148(4) | -0.0142(3) | -0.0147(3) |
| | $D_{2233}$ | -0.0133(3) | -0.0092(3) | -0.0080(2) | -0.0074(3) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.0342(7) | 0.0385(8) | 0.0362(6) | 0.0389(6) |
| | $U_{11}$ | 0.0115(2) | 0.0155(3) | 0.0196(2) | 0.0250(3) |
| | $U_{22}$ | 0.0104(2) | 0.0143(2) | 0.0182(2) | 0.0238(2) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.2076(9) | 0.2068(10) | 0.2072(7) | 0.2141(7) |
| | x | 0.18429(1) | 0.18435(2) | 0.18435(1) | 0.18420(1) |
| | $U_{11}$ | 0.00969(6) | 0.01346(8) | 0.01805(6) | 0.02322(7) |
| | $U_{12}$ | 0.00004(4) | -0.00018(6) | -0.00049(5) | -0.00109(5) |
| Sn/Ga(3) 24k | y | 0.31240(2) | 0.31236(2) | 0.31227(2) | 0.31230(2) |
| | z | 0.11873(2) | 0.11875(2) | 0.11876(2) | 0.11858(2) |
| | $U_{11}$ | 0.01226(8) | 0.0162(1) | 0.02104(9) | 0.0266(1) |
| | $U_{22}$ | 0.00922(8) | 0.0128(1) | 0.01712(8) | 0.02201(9) |
| | $U_{33}$ | 0.00884(8) | 0.0121(1) | 0.01628(8) | 0.02121(9) |
| | $U_{23}$ | -0.00116(5) | -0.00131(7) | -0.00171(6) | -0.00184(7) |

**Table 4 Crystallographic details and refined parameters from refinement of "Anharmonic"-model against x-ray data of p-1BGS**

| p-1BGS "*Anharmonic model*" | | Radiation source: | | | X-ray |
|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 400 |
| $N_{par}$ | | 23 | 23 | 23 | 23 |
| $N_{obs}$ | | 1452 | 1456 | 1464 | 1472 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 1130 | 1055 | 938 | 823 |
| $R_F$ | | 3.92 | 4.2 | 4.76 | 5.82 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 2.68 | 2.32 | 2.25 | 2.29 |
| $R_{wF}$ | | 3.77 | 2.85 | 3.76 | 2.95 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 3.09 | 2.51 | 2.38 | 2.45 |
| $R_{internal}$ | | 3.90 | 4.05 | 4.41 | 4.89 |
| extinction | | 0.030(8) | 0.052(6) | 0.125(9) | 0.141(7) |
| Ba(1) 2a | $U_{11}$ | 0.0109(1) | 0.01647(10) | 0.0218(1) | 0.0281(1) |
| Ba(2) 6d | $U_{11}$ | 0.0213(7) | 0.0285(6) | 0.0357(9) | 0.0446(8) |
| | $U_{22}$ | 0.1302(8) | 0.1373(7) | 0.144(1) | 0.1553(9) |
| | $C_{122}$ | 0.0072(2) | 0.0061(2) | 0.0057(2) | 0.0058(2) |
| | $D_{1111}$ | 0.00010(6) | 0.00005(6) | 0.0000(1) | 0.0001(1) |
| | $D_{1122}$ | -0.00013(6) | -0.00016(6) | -0.00037(8) | -0.00039(8) |
| | $D_{2222}$ | -0.0194(4) | -0.0156(3) | -0.0146(4) | -0.0142(4) |
| | $D_{2233}$ | -0.0139(3) | -0.0103(2) | -0.0084(3) | -0.0082(3) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.0412(9) | 0.0395(7) | 0.0419(9) | 0.0367(7) |
| | $U_{11}$ | 0.0125(3) | 0.0161(2) | 0.0209(3) | 0.0255(3) |
| | $U_{22}$ | 0.0121(2) | 0.0157(2) | 0.0199(2) | 0.0240(2) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.217(1) | 0.2175(9) | 0.216(1) | 0.2173(9) |
| | x | 0.18411(2) | 0.18414(1) | 0.18418(2) | 0.18420(1) |
| | $U_{11}$ | 0.01039(8) | 0.01460(7) | 0.01861(9) | 0.02382(8) |
| | $U_{12}$ | -0.00009(5) | -0.00041(5) | -0.00077(7) | -0.00109(6) |
| Sn/Ga(3) 24k | y | 0.31240(2) | 0.31233(2) | 0.31229(2) | 0.31234(2) |
| | z | 0.11841(2) | 0.11842(2) | 0.11843(2) | 0.11851(2) |
| | $U_{11}$ | 0.0125(1) | 0.01687(9) | 0.0213(1) | 0.0271(1) |
| | $U_{22}$ | 0.00981(10) | 0.01395(8) | 0.0176(1) | 0.0225(1) |
| | $U_{33}$ | 0.00950(10) | 0.01333(8) | 0.0170(1) | 0.0218(1) |
| | $U_{23}$ | -0.00090(7) | -0.00120(6) | -0.00149(9) | -0.00186(7) |

**Table 5 Crystallographic details and refined parameters from refinement of "Anharmonic"-model against neutron data of n-1BGS**

| n-1BGS "*Anharmonic model*" | | Radiation source: | | | Neutron | | |
|---|---|---|---|---|---|---|---|
| Temperature | | 10 | 100 | 200 | 300 | 400 | 500 |
| $N_{par}$ | | 23 | 23 | 23 | 23 | 23 | 23 |
| $N_{obs}$ | | 459 | 456 | 459 | 390 | 395 | 259 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 357 | 346 | 335 | 297 | 309 | 198 |
| $R_F$ | | 5.5 | 5.33 | 6.36 | 5.15 | 5.1 | 6.26 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 2.97 | 2.77 | 3.07 | 2.50 | 2.56 | 3.68 |
| $R_{wF}$ | | 3.41 | 3.08 | 3.21 | 2.72 | 2.98 | 4.00 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 3.14 | 2.77 | 2.79 | 2.21 | 2.73 | 3.70 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.012(3) | 0.11(2) | 0.10(2) | 0.006(2) | 0.10(3) | 0.02(4) |
| Ba(1) 2a | $U_{11}$ | 0.0045(5) | 0.0079(5) | 0.0136(5) | 0.0190(6) | 0.0243(5) | 0.029(1) |
| Ba(2) 6d | $U_{11}$ | 0.020(3) | 0.023(3) | 0.025(3) | 0.030(3) | 0.042(3) | 0.040(7) |
| | $U_{22}$ | 0.118(2) | 0.123(2) | 0.131(3) | 0.137(3) | 0.155(3) | 0.169(8) |
| | $C_{122}$ | 0.0086(7) | 0.0065(7) | 0.0054(7) | 0.0046(7) | 0.0054(8) | 0.006(2) |
| | $D_{1111}$ | 0.0013(6) | 0.0011(6) | 0.0002(5) | -0.0001(6) | 0.0005(6) | 0.001(1) |
| | $D_{1122}$ | -0.0005(3) | -0.0002(3) | 0.0002(3) | -0.0000(3) | -0.0006(3) | -0.0015(8) |
| | $D_{2222}$ | -0.026(1) | -0.019(1) | -0.017(1) | -0.013(1) | -0.014(1) | -0.012(4) |
| | $D_{2233}$ | -0.021(1) | -0.013(1) | -0.010(1) | -0.010(1) | -0.008(1) | -0.008(3) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.042(5) | 0.050(4) | 0.050(5) | 0.032(4) | 0.055(4) | 0.055(7) |
| | $U_{11}$ | 0.0069(6) | 0.0092(6) | 0.0127(6) | 0.0171(6) | 0.0231(6) | 0.027(1) |
| | $U_{22}$ | 0.0062(4) | 0.0079(4) | 0.0118(4) | 0.0165(4) | 0.0213(4) | 0.0258(9) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.200(7) | 0.202(6) | 0.200(6) | 0.215(6) | 0.205(6) | 0.21(1) |
| | x | 0.18391(4) | 0.18390(3) | 0.18393(4) | 0.18400(4) | 0.18390(4) | 0.18377(7) |
| | $U_{11}$ | 0.0055(2) | 0.0079(2) | 0.0121(2) | 0.0159(2) | 0.0219(3) | 0.0252(5) |
| | $U_{12}$ | 0.0000(1) | -0.0001(1) | -0.0003(2) | -0.0009(1) | -0.0010(2) | -0.0016(3) |
| Sn/Ga(3) 24k | y | 0.31212(5) | 0.31214(5) | 0.31207(5) | 0.31202(5) | 0.31208(5) | 0.31211(10) |
| | z | 0.11839(5) | 0.11838(4) | 0.11839(5) | 0.11844(5) | 0.11823(4) | 0.11799(9) |
| | $U_{11}$ | 0.0073(3) | 0.0102(3) | 0.0146(3) | 0.0185(3) | 0.0246(3) | 0.0288(7) |
| | $U_{22}$ | 0.0050(3) | 0.0075(3) | 0.0115(3) | 0.0152(3) | 0.0210(3) | 0.0252(7) |
| | $U_{33}$ | 0.0046(3) | 0.0068(3) | 0.0104(3) | 0.0145(3) | 0.0200(3) | 0.0229(6) |
| | $U_{23}$ | -0.0005(2) | -0.0007(2) | -0.0011(2) | -0.0012(2) | -0.0016(2) | -0.0019(5) |

**Table 6 Crystallographic details and refined parameters from refinement of "Anharmonic"-model against neutron data of p-1BGS**

| p-1BGS "*Anharmonic model*" | | Radiation source: | | | Neutron | | | |
|---|---|---|---|---|---|---|---|---|
| Temperature | | 10 | 50 | 100 | 200 | 300 | 300 | 400 |
| $N_{par}$ | | 23 | 23 | 23 | 23 | 23 | 23 | 23 |
| $N_{obs}$ | | 426 | 426 | 429 | 431 | 373 | 356 | 396 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 349 | 348 | 339 | 336 | 292 | 279 | 307 |
| $R_F$ | | 5.20 | 5.18 | 5.23 | 5.36 | 4.81 | 6.41 | 5.17 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 3.12 | 3.32 | 3.07 | 3.13 | 2.70 | 3.77 | 2.78 |
| $R_{wF}$ | | 4.11 | 4.06 | 3.85 | 3.54 | 3.14 | 3.54 | 3.22 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 3.91 | 3.92 | 3.65 | 3.34 | 2.94 | 3.23 | 2.86 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.016(3) | 0.015(3) | 0.015(3) | 0.013(3) | 0.013(3) | 0.013(3) | 0.012(3) |
| Ba(1) 2a | $U_{11}$ | 0.0050(5) | 0.0058(5) | 0.0086(5) | 0.0139(5) | 0.0186(6) | 0.0177(8) | 0.0238(6) |
| Ba(2) 6d | $U_{11}$ | 0.023(3) | 0.023(3) | 0.025(4) | 0.037(4) | 0.035(4) | 0.033(5) | 0.039(4) |
| | $U_{22}$ | 0.126(2) | 0.129(3) | 0.131(3) | 0.138(3) | 0.150(4) | 0.148(5) | 0.159(4) |
| | $C_{122}$ | 0.0092(9) | 0.0083(9) | 0.0064(8) | 0.0054(8) | 0.0058(8) | 0.005(1) | 0.0052(8) |
| | $D_{1111}$ | 0.0019(7) | 0.0016(7) | 0.0013(7) | 0.0020(9) | 0.0007(6) | 0.0003(9) | 0.0004(7) |
| | $D_{1122}$ | -0.0008(4) | -0.0007(4) | -0.0005(4) | -0.0004(4) | -0.0007(4) | -0.0002(5) | -0.0006(4) |
| | $D_{2222}$ | -0.027(2) | -0.023(2) | -0.021(2) | -0.016(2) | -0.014(2) | -0.013(2) | -0.013(2) |
| | $D_{2233}$ | -0.023(1) | -0.018(1) | -0.013(1) | -0.010(1) | -0.009(1) | -0.011(2) | -0.010(1) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.063(5) | 0.062(5) | 0.063(4) | 0.064(4) | 0.059(4) | 0.059(5) | 0.059(4) |
| | $U_{11}$ | 0.0066(6) | 0.0072(6) | 0.0093(6) | 0.0134(6) | 0.0176(6) | 0.0178(9) | 0.0218(7) |
| | $U_{22}$ | 0.0063(5) | 0.0074(5) | 0.0086(4) | 0.0120(4) | 0.0165(4) | 0.0152(6) | 0.0207(5) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.190(8) | 0.197(8) | 0.197(8) | 0.199(7) | 0.204(7) | 0.213(8) | 0.202(7) |
| | x | 0.18379(4) | 0.18380(4) | 0.18379(4) | 0.18385(4) | 0.18384(4) | 0.18386(5) | 0.18387(4) |
| | $U_{11}$ | 0.0060(3) | 0.0067(3) | 0.0085(3) | 0.0125(2) | 0.0168(3) | 0.0161(3) | 0.0214(3) |
| | $U_{12}$ | -0.0002(2) | -0.0001(2) | -0.0003(1) | -0.0006(1) | -0.0009(2) | -0.0008(2) | -0.0010(2) |
| Sn/Ga(3) 24k | y | 0.31199(6) | 0.31202(6) | 0.31197(5) | 0.31198(5) | 0.31197(5) | 0.31207(7) | 0.31199(5) |
| | z | 0.11805(5) | 0.11809(5) | 0.11809(5) | 0.11813(5) | 0.11809(5) | 0.11817(6) | 0.11825(5) |
| | $U_{11}$ | 0.0079(3) | 0.0083(3) | 0.0102(3) | 0.0145(3) | 0.0192(3) | 0.0189(5) | 0.0244(4) |
| | $U_{22}$ | 0.0054(3) | 0.0066(3) | 0.0082(3) | 0.0120(3) | 0.0165(3) | 0.0160(4) | 0.0204(3) |
| | $U_{33}$ | 0.0056(3) | 0.0063(3) | 0.0080(3) | 0.0115(3) | 0.0160(3) | 0.0153(4) | 0.0196(3) |
| | $U_{23}$ | -0.0004(2) | -0.0005(2) | -0.0005(2) | -0.0009(2) | -0.0014(2) | -0.0013(3) | -0.0018(2) |

**Table 7 Crystallographic details and refined parameters from refinement of "Harmonic"-model against x-ray data of n-1BGS**

| n-1BGS "*Harmonic model*" | | Radiation source: | | | X-ray |
|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 400 |
| $N_{par}$ | | 18 | 18 | 18 | 18 |
| $N_{obs}$ | | 1545 | 1564 | 1559 | 1583 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 1221 | 1136 | 1014 | 922 |
| $R_F$ | | 7.00 | 6.11 | 6.26 | 6.88 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 5.81 | 4.49 | 3.90 | 3.87 |
| $R_{wF}$ | | 8.74 | 7.17 | 5.68 | 5.39 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 8.66 | 6.50 | 5.53 | 5.20 |
| $R_{internal}$ | | 2.74 | 2.86 | 2.94 | 3.11 |
| extinction | | 0.03(2) | 0.04(1) | 0.05(1) | 0.08(1) |
| Ba(1) 2a | $U_{11}$ | 0.0104(2) | 0.0156(2) | 0.0214(2) | 0.0278(2) |
| Ba(2) 6d | $U_{11}$ | 0.0141(8) | 0.0227(8) | 0.0313(7) | 0.0411(8) |
| | $U_{22}$ | 0.210(3) | 0.194(2) | 0.196(2) | 0.204(2) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.038(2) | 0.042(1) | 0.039(1) | 0.043(1) |
| | $U_{11}$ | 0.0121(6) | 0.0165(5) | 0.0205(5) | 0.0261(5) |
| | $U_{22}$ | 0.0107(4) | 0.0145(4) | 0.0185(3) | 0.0242(3) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.206(2) | 0.205(2) | 0.205(1) | 0.213(1) |
| | x | 0.18428(4) | 0.18432(3) | 0.18432(3) | 0.18420(2) |
| | $U_{11}$ | 0.0095(2) | 0.0133(1) | 0.0179(1) | 0.0231(1) |
| | $U_{12}$ | 0.0001(1) | -0.0002(1) | -0.00049(9) | -0.00103(10) |
| Sn/Ga(3) 24k | y | 0.31230(5) | 0.31230(4) | 0.31220(3) | 0.31222(3) |
| | z | 0.11870(5) | 0.11872(4) | 0.11874(3) | 0.11852(3) |
| | $U_{11}$ | 0.0121(2) | 0.0163(2) | 0.0211(2) | 0.0267(2) |
| | $U_{22}$ | 0.0091(2) | 0.0126(2) | 0.0169(2) | 0.0218(2) |
| | $U_{33}$ | 0.0088(2) | 0.0120(2) | 0.0162(2) | 0.0210(2) |
| | $U_{23}$ | -0.0010(1) | -0.0012(1) | -0.0016(1) | -0.0017(1) |

**Table 8 Crystallographic details and refined parameters from refinement of "Harmonic"-model against x-ray data of p-1BGS**

| p-1BGS "*Harmonic model*" | | Radiation source: | | | X-ray |
|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 400 |
| $N_{par}$ | | 18 | 18 | 18 | 18 |
| $N_{obs}$ | | 1452 | 1456 | 1464 | 1472 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 1130 | 1055 | 938 | 823 |
| $R_F$ | | 7.31 | 6.4 | 6.61 | 7.3 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 6.02 | 4.63 | 4.16 | 3.81 |
| $R_{wF}$ | | 9.22 | 6.64 | 6.35 | 5.34 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 8.92 | 6.5 | 5.62 | 5.09 |
| $R_{internal}$ | | 3.9 | 4.05 | 4.41 | 4.89 |
| extinction | | 0.01(2) | 0.04(1) | 0.11(2) | 0.13(1) |
| Ba(1) 2a | $U_{11}$ | 0.0110(3) | 0.0166(2) | 0.0220(2) | 0.0284(2) |
| Ba(2) 6d | $U_{11}$ | 0.016(1) | 0.0248(9) | 0.0332(10) | 0.0418(9) |
| | $U_{22}$ | 0.220(4) | 0.204(2) | 0.202(2) | 0.208(2) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.042(2) | 0.042(2) | 0.045(1) | 0.039(1) |
| | $U_{11}$ | 0.0130(7) | 0.0167(5) | 0.0217(6) | 0.0259(5) |
| | $U_{22}$ | 0.0122(5) | 0.0160(4) | 0.0202(4) | 0.0244(4) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.217(3) | 0.217(2) | 0.215(2) | 0.216(2) |
| | x | 0.18411(4) | 0.18414(3) | 0.18419(3) | 0.18419(3) |
| | $U_{11}$ | 0.0102(2) | 0.0145(2) | 0.0185(2) | 0.0237(1) |
| | $U_{12}$ | -0.0001(1) | -0.0004(1) | -0.0008(1) | -0.0012(1) |
| Sn/Ga(3) 24k | y | 0.31231(5) | 0.31227(4) | 0.31223(4) | 0.31228(4) |
| | z | 0.11836(5) | 0.11838(4) | 0.11839(4) | 0.11848(3) |
| | $U_{11}$ | 0.0123(3) | 0.0168(2) | 0.0213(2) | 0.0271(2) |
| | $U_{22}$ | 0.0097(2) | 0.0138(2) | 0.0174(2) | 0.0222(2) |
| | $U_{33}$ | 0.0094(2) | 0.0132(2) | 0.0168(2) | 0.0215(2) |
| | $U_{23}$ | -0.0007(2) | -0.0010(1) | -0.0013(1) | -0.0018(1) |

**Table 9 Crystallographic details and refined parameters from refinement of "Harmonic"-model against neutron data of n-1BGS**

| n-1BGS "*Harmonic model*" | | Radiation source: | | Neutron | | | |
|---|---|---|---|---|---|---|---|
| Temperature | | 10 | 100 | 200 | 300 | 400 | 500 |
| $N_{par}$ | | 18 | 18 | 18 | 18 | 18 | 18 |
| $N_{obs}$ | | 459 | 456 | 459 | 390 | 395 | 259 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 357 | 346 | 335 | 297 | 309 | 198 |
| $R_F$ | | 8.85 | 6.98 | 7.37 | 6.04 | 5.9 | 6.75 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 6.25 | 4.52 | 4.06 | 3.36 | 3.24 | 4.04 |
| $R_{wF}$ | | 6.95 | 4.81 | 4.11 | 3.47 | 3.60 | 4.29 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 6.79 | 4.62 | 3.78 | 3.08 | 3.37 | 4 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.014(5) | 0.11(4) | 0.10(3) | 0.05(3) | 0.09(3) | 0.00(4) |
| Ba(1) 2a | $U_{11}$ | 0.006(1) | 0.0090(7) | 0.0146(7) | 0.0202(7) | 0.0249(7) | 0.029(1) |
| Ba(2) 6d | $U_{11}$ | 0.004(4) | 0.011(3) | 0.019(2) | 0.026(2) | 0.038(2) | 0.038(4) |
| | $U_{22}$ | 0.24(1) | 0.201(6) | 0.190(5) | 0.191(5) | 0.202(4) | 0.209(7) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.05(1) | 0.059(7) | 0.056(6) | 0.046(6) | 0.058(5) | 0.057(7) |
| | $U_{11}$ | 0.007(1) | 0.0091(9) | 0.0127(8) | 0.0168(8) | 0.0231(7) | 0.027(1) |
| | $U_{22}$ | 0.0045(8) | 0.0067(6) | 0.0111(5) | 0.0153(5) | 0.0208(5) | 0.0254(10) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.20(1) | 0.199(10) | 0.198(8) | 0.204(7) | 0.208(8) | 0.21(1) |
| | x | 0.18390(8) | 0.18390(5) | 0.18395(5) | 0.18401(5) | 0.18394(4) | 0.18378(8) |
| | $U_{11}$ | 0.0058(4) | 0.0081(3) | 0.0123(3) | 0.0164(3) | 0.0219(3) | 0.0252(5) |
| | $U_{12}$ | 0.0001(3) | -0.0000(2) | -0.0003(2) | -0.0008(2) | -0.0010(2) | -0.0017(3) |
| Sn/Ga(3) 24k | y | 0.3122(1) | 0.31220(7) | 0.31213(6) | 0.31209(6) | 0.31210(6) | 0.31216(10) |
| | z | 0.11835(10) | 0.11837(7) | 0.11839(6) | 0.11842(6) | 0.11824(5) | 0.11801(10) |
| | $U_{11}$ | 0.0076(6) | 0.0105(4) | 0.0148(4) | 0.0188(4) | 0.0248(4) | 0.0290(8) |
| | $U_{22}$ | 0.0042(6) | 0.0069(4) | 0.0110(4) | 0.0146(4) | 0.0206(4) | 0.0247(7) |
| | $U_{33}$ | 0.0039(5) | 0.0063(4) | 0.0100(4) | 0.0141(4) | 0.0195(3) | 0.0224(6) |
| | $U_{23}$ | 0.0002(4) | -0.0003(3) | -0.0009(3) | -0.0010(3) | -0.0016(2) | -0.0018(5) |

**Table 10 Crystallographic details and refined parameters from refinement of "Harmonic"-model against neutron data of p-1BGS**

| p-1BGS "*Harmonic model*" | | Radiation source: | | | Neutron | | | |
|---|---|---|---|---|---|---|---|---|
| Temperature | | 10 | 50 | 100 | 200 | **300** | 300 | 400 |
| $N_{par}$ | | 18 | 18 | 18 | 18 | 18 | 18 | 18 |
| $N_{obs}$ | | 426 | 426 | 429 | 431 | 373 | 356 | 396 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 349 | 348 | 339 | 336 | 292 | 279 | 307 |
| $R_F$ | | 8.35 | 7.53 | 6.83 | 6.29 | 5.69 | 7.17 | 5.85 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 6.15 | 5.63 | 4.68 | 4.03 | 3.55 | 4.53 | 3.42 |
| $R_{wF}$ | | 7.52 | 6.39 | 5.42 | 4.33 | 3.84 | 4.05 | 3.77 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 7.39 | 6.28 | 5.27 | 4.16 | 3.65 | 3.81 | 3.47 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.016(6) | 0.015(5) | 0.014(5) | 0.012(4) | 0.012(4) | 0.012(4) | 0.010(4) |
| Ba(1) 2a | $U_{11}$ | 0.0058(10) | 0.0063(9) | 0.0091(8) | 0.0143(7) | 0.0191(7) | 0.0185(9) | 0.0246(7) |
| Ba(2) 6d | $U_{11}$ | 0.005(3) | 0.009(3) | 0.013(3) | 0.023(2) | 0.030(2) | 0.028(3) | 0.036(2) |
| | $U_{22}$ | 0.25(1) | 0.229(8) | 0.212(6) | 0.196(5) | 0.198(4) | 0.196(5) | 0.205(4) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.064(8) | 0.063(7) | 0.066(6) | 0.066(5) | 0.061(5) | 0.062(6) | 0.061(5) |
| | $U_{11}$ | 0.008(1) | 0.008(1) | 0.0098(9) | 0.0138(8) | 0.0176(7) | 0.0180(10) | 0.0218(8) |
| | $U_{22}$ | 0.0053(8) | 0.0064(7) | 0.0078(6) | 0.0114(5) | 0.0160(5) | 0.0144(7) | 0.0201(5) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.20(1) | 0.21(1) | 0.20(1) | 0.203(8) | 0.206(8) | 0.213(9) | 0.203(8) |
| | x | 0.18384(7) | 0.18384(6) | 0.18383(5) | 0.18387(5) | 0.18387(5) | 0.18392(6) | 0.18392(4) |
| | $U_{11}$ | 0.0058(5) | 0.0065(4) | 0.0083(4) | 0.0125(3) | 0.0168(3) | 0.0162(4) | 0.0216(3) |
| | $U_{12}$ | -0.0000(3) | 0.0000(2) | -0.0002(2) | -0.0005(2) | -0.0008(2) | -0.0008(2) | -0.0011(2) |
| Sn/Ga(3) 24k | y | 0.3120(1) | 0.31203(9) | 0.31198(7) | 0.31200(6) | 0.31198(6) | 0.31211(8) | 0.31202(6) |
| | z | 0.11805(9) | 0.11807(8) | 0.11810(7) | 0.11813(6) | 0.11810(6) | 0.11818(7) | 0.11825(6) |
| | $U_{11}$ | 0.0080(6) | 0.0085(5) | 0.0104(4) | 0.0147(4) | 0.0194(4) | 0.0190(5) | 0.0245(4) |
| | $U_{22}$ | 0.0049(6) | 0.0061(5) | 0.0078(4) | 0.0116(4) | 0.0161(4) | 0.0155(5) | 0.0199(4) |
| | $U_{33}$ | 0.0048(5) | 0.0058(4) | 0.0076(4) | 0.0112(3) | 0.0156(3) | 0.0149(5) | 0.0191(4) |
| | $U_{23}$ | -0.0004(4) | -0.0004(3) | -0.0004(3) | -0.0009(3) | -0.0013(3) | -0.0014(3) | -0.0018(3) |

**Table 11 Crystallographic details and refined parameters from refinement of "24k"-model against x-ray data of n-1BGS**

| n-1BGS "*24k model*" | | Radiation source: | | | X-ray |
|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 400 |
| $N_{par}$ | | 19 | 19 | 19 | 19 |
| $N_{obs}$ | | 1545 | 1564 | 1559 | 1583 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 1221 | 1136 | 1014 | 922 |
| $R_F$ | | 5.71 | 5.59 | 6.06 | 6.57 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 4.45 | 3.96 | 3.62 | 3.53 |
| $R_{wF}$ | | 6.14 | 5.89 | 4.79 | 4.63 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 6.03 | 5.07 | 4.60 | 4.36 |
| $R_{internal}$ | | 2.74 | 2.86 | 2.94 | 3.11 |
| extinction | | 0.05(1) | 0.06(1) | 0.063(9) | 0.094(9) |
| Ba(1) 2a | $U_{11}$ | 0.0103(2) | 0.0156(2) | 0.0214(2) | 0.0278(2) |
| Ba(2) 6d | x | 0.2538(2) | 0.2534(3) | 0.2534(2) | 0.2535(2) |
| | y | 0.5404(1) | 0.5380(1) | 0.5377(1) | 0.5380(1) |
| | $U_{11}$ | 0.0317(4) | 0.0393(5) | 0.0476(5) | 0.0561(5) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.035(1) | 0.038(1) | 0.0360(9) | 0.0392(9) |
| | $U_{11}$ | 0.0118(4) | 0.0160(4) | 0.0199(4) | 0.0254(4) |
| | $U_{22}$ | 0.0105(3) | 0.0142(3) | 0.0181(3) | 0.0238(3) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.207(2) | 0.207(1) | 0.207(1) | 0.214(1) |
| | x | 0.18426(3) | 0.18433(3) | 0.18434(2) | 0.18422(2) |
| | $U_{11}$ | 0.0097(1) | 0.0135(1) | 0.0181(1) | 0.0233(1) |
| | $U_{12}$ | 0.00001(8) | -0.00018(8) | -0.00051(8) | -0.00108(8) |
| Sn/Ga(3) 24k | y | 0.31238(3) | 0.31235(3) | 0.31227(3) | 0.31230(3) |
| | z | 0.11869(3) | 0.11869(3) | 0.11870(3) | 0.11850(3) |
| | $U_{11}$ | 0.0124(2) | 0.0164(2) | 0.0213(2) | 0.0268(2) |
| | $U_{22}$ | 0.0093(1) | 0.0128(2) | 0.0173(1) | 0.0222(1) |
| | $U_{33}$ | 0.0089(1) | 0.0121(1) | 0.0162(1) | 0.0211(1) |
| | $U_{23}$ | -0.0012(1) | -0.0013(1) | -0.0017(1) | -0.0019(1) |

**Table 12 Crystallographic details and refined parameters from refinement of "24k"-model against x-ray data of p-1BGS**

| p-1BGS "*24k model*" | | Radiation source: | | | X-ray |
|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 400 |
| $N_{par}$ | | 19 | 19 | 19 | 19 |
| $N_{obs}$ | | 1452 | 1456 | 1464 | 1472 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 1130 | 1055 | 938 | 823 |
| $R_F$ | | 5.74 | 5.82 | 6.13 | 7.02 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 4.45 | 3.91 | 3.55 | 3.43 |
| $R_{wF}$ | | 5.99 | 4.91 | 5.16 | 4.42 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 5.57 | 4.71 | 4.20 | 4.07 |
| $R_{internal}$ | | 3.90 | 4.05 | 4.41 | 4.89 |
| extinction | | 0.03(1) | 0.06(1) | 0.13(1) | 0.15(1) |
| Ba(1) 2a | $U_{11}$ | 0.0110(2) | 0.0166(2) | 0.0219(2) | 0.0283(2) |
| Ba(2) 6d | x | 0.2543(2) | 0.2539(2) | 0.2538(3) | 0.2538(2) |
| | y | 0.5409(2) | 0.5386(1) | 0.5378(1) | 0.5380(1) |
| | $U_{11}$ | 0.0335(5) | 0.0424(5) | 0.0499(6) | 0.0585(5) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.040(1) | 0.038(1) | 0.042(1) | 0.0362(10) |
| | $U_{11}$ | 0.0126(4) | 0.0162(4) | 0.0213(5) | 0.0257(4) |
| | $U_{22}$ | 0.0120(3) | 0.0155(3) | 0.0197(3) | 0.0239(3) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.218(2) | 0.219(2) | 0.216(2) | 0.217(1) |
| | x | 0.18410(3) | 0.18413(2) | 0.18419(2) | 0.18420(2) |
| | $U_{11}$ | 0.0105(1) | 0.0148(1) | 0.0187(1) | 0.0239(1) |
| | $U_{12}$ | -0.00013(8) | -0.00043(8) | -0.00076(9) | -0.00113(8) |
| Sn/Ga(3) 24k | y | 0.31241(4) | 0.31234(3) | 0.31230(3) | 0.31234(3) |
| | z | 0.11837(3) | 0.11836(3) | 0.11836(3) | 0.11845(3) |
| | $U_{11}$ | 0.0126(2) | 0.0170(2) | 0.0215(2) | 0.0273(2) |
| | $U_{22}$ | 0.0099(2) | 0.0141(1) | 0.0178(2) | 0.0226(2) |
| | $U_{33}$ | 0.0095(2) | 0.0133(1) | 0.0169(2) | 0.0217(2) |
| | $U_{23}$ | -0.0009(1) | -0.0013(1) | -0.0015(1) | -0.0020(1) |

**Table 13 Crystallographic details and refined parameters from refinement of "24k"-model against neutron data of n-1BGS**

| n-1BGS "*24k model*" | | Radiation source: | | Neutron | | | |
|---|---|---|---|---|---|---|---|
| Temperature | | 10 | 100 | 200 | 300 | 400 | 500 |
| $N_{par}$ | | 19 | 19 | 19 | 19 | 19 | 19 |
| $N_{obs}$ | | 459 | 456 | 459 | 390 | 395 | 259 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 357 | 346 | 335 | 297 | 309 | 198 |
| $R_F$ | | 5.97 | 5.96 | 6.78 | 5.41 | 5.57 | 6.83 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 3.47 | 3.3 | 3.55 | 2.82 | 3.02 | 4.08 |
| $R_{wF}$ | | 3.8 | 3.53 | 3.61 | 2.98 | 3.4 | 4.3 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 3.53 | 3.24 | 3.24 | 2.53 | 3.16 | 4 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.013(3) | 0.12(3) | 0.11(3) | 0.06(2) | 0.12(3) | 0.03(4) |
| Ba(1) 2a | $U_{11}$ | 0.0048(5) | 0.0080(5) | 0.0135(6) | 0.0188(6) | 0.0243(6) | 0.029(1) |
| Ba(2) 6d | x | 0.2549(4) | 0.2540(5) | 0.2536(6) | 0.2534(6) | 0.2535(6) | 0.253(1) |
| | y | 0.5452(3) | 0.5410(3) | 0.5391(4) | 0.5386(4) | 0.5394(4) | 0.5402(7) |
| | $U_{11}$ | 0.0186(9) | 0.028(1) | 0.036(1) | 0.041(1) | 0.052(2) | 0.053(3) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.046(5) | 0.052(5) | 0.050(5) | 0.032(5) | 0.054(4) | 0.052(7) |
| | $U_{11}$ | 0.0077(6) | 0.0099(6) | 0.0135(7) | 0.0176(7) | 0.0237(7) | 0.027(1) |
| | $U_{22}$ | 0.0054(4) | 0.0076(4) | 0.0117(5) | 0.0165(5) | 0.0214(5) | 0.0265(10) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.199(8) | 0.202(7) | 0.202(7) | 0.218(6) | 0.206(7) | 0.22(1) |
| | x | 0.18392(4) | 0.18391(4) | 0.18395(4) | 0.18402(4) | 0.18390(4) | 0.18379(7) |
| | $U_{11}$ | 0.0056(2) | 0.0079(2) | 0.0121(2) | 0.0158(2) | 0.0218(3) | 0.0251(5) |
| | $U_{12}$ | 0.0000(2) | -0.0001(2) | -0.0003(2) | -0.0009(2) | -0.0011(2) | -0.0018(3) |
| Sn/Ga(3) 24k | y | 0.31206(6) | 0.31211(5) | 0.31204(6) | 0.31200(5) | 0.31204(5) | 0.3121(1) |
| | z | 0.11837(5) | 0.11836(5) | 0.11838(5) | 0.11843(5) | 0.11821(5) | 0.11799(10) |
| | $U_{11}$ | 0.0076(3) | 0.0104(3) | 0.0148(4) | 0.0187(4) | 0.0248(4) | 0.0286(8) |
| | $U_{22}$ | 0.0053(3) | 0.0077(3) | 0.0116(4) | 0.0153(3) | 0.0212(3) | 0.0255(7) |
| | $U_{33}$ | 0.0047(3) | 0.0070(3) | 0.0107(3) | 0.0148(3) | 0.0202(3) | 0.0236(6) |
| | $U_{23}$ | -0.0007(2) | -0.0010(2) | -0.0014(2) | -0.0014(2) | -0.0018(2) | -0.0023(5) |

**Table 14 Crystallographic details and refined parameters from refinement of "24k"-model against neutron data of p-1BGS**

| p-1BGS "*24k model*" | | Radiation source: | | | Neutron | | | |
|---|---|---|---|---|---|---|---|---|
| Temperature | | 10 | 50 | 100 | 200 | 200 | 300 | 400 |
| $N_{par}$ | | 19 | 19 | 19 | 19 | 19 | 19 | 19 |
| $N_{obs}$ | | 426 | 426 | 429 | 431 | 431 | 356 | 396 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 349 | 348 | 339 | 336 | 336 | 279 | 307 |
| $R_F$ | | 5.47 | 5.65 | 5.66 | 5.72 | 5.72 | 6.73 | 5.65 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 3.49 | 3.85 | 3.53 | 3.43 | 3.43 | 4 | 3.28 |
| $R_{wF}$ | | 4.44 | 4.45 | 4.27 | 3.82 | 3.82 | 3.82 | 3.64 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 4.26 | 4.33 | 4.08 | 3.62 | 3.62 | 3.5 | 3.33 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.018(4) | 0.017(4) | 0.016(4) | 0.014(3) | 0.014(3) | 0.013(3) | 0.013(4) |
| Ba(1) 2a | $U_{11}$ | 0.0050(6) | 0.0057(6) | 0.0087(6) | 0.0139(6) | 0.0139(6) | 0.0175(8) | 0.0235(7) |
| Ba(2) 6d | x | 0.2548(4) | 0.2544(5) | 0.2538(5) | 0.2533(6) | 0.2533(6) | 0.2529(8) | 0.2532(7) |
| | y | 0.5459(3) | 0.5440(4) | 0.5419(4) | 0.5398(4) | 0.5398(4) | 0.5393(5) | 0.5395(4) |
| | $U_{11}$ | 0.019(1) | 0.023(1) | 0.029(1) | 0.038(1) | 0.038(1) | 0.044(2) | 0.052(2) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.065(5) | 0.062(5) | 0.064(5) | 0.064(4) | 0.064(4) | 0.058(6) | 0.057(5) |
| | $U_{11}$ | 0.0078(7) | 0.0082(7) | 0.0101(7) | 0.0141(7) | 0.0141(7) | 0.0183(9) | 0.0225(7) |
| | $U_{22}$ | 0.0054(5) | 0.0068(5) | 0.0082(5) | 0.0118(5) | 0.0118(5) | 0.0154(6) | 0.0209(5) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.190(9) | 0.197(9) | 0.196(8) | 0.197(7) | 0.197(7) | 0.214(9) | 0.204(8) |
| | x | 0.18380(4) | 0.18380(4) | 0.18379(4) | 0.18386(4) | 0.18386(4) | 0.18387(5) | 0.18387(4) |
| | $U_{11}$ | 0.0061(3) | 0.0068(3) | 0.0086(3) | 0.0126(3) | 0.0126(3) | 0.0160(3) | 0.0214(3) |
| | $U_{12}$ | -0.0002(2) | -0.0002(2) | -0.0004(2) | -0.0007(2) | -0.0007(2) | -0.0009(2) | -0.0012(2) |
| Sn/Ga(3) 24k | y | 0.31192(6) | 0.31192(6) | 0.31191(6) | 0.31196(6) | 0.31196(6) | 0.31205(7) | 0.31193(6) |
| | z | 0.11805(6) | 0.11807(6) | 0.11807(5) | 0.11809(5) | 0.11809(5) | 0.11815(7) | 0.11823(5) |
| | $U_{11}$ | 0.0080(3) | 0.0085(3) | 0.0104(3) | 0.0147(3) | 0.0147(3) | 0.0191(5) | 0.0246(4) |
| | $U_{22}$ | 0.0056(4) | 0.0068(4) | 0.0083(4) | 0.0120(3) | 0.0120(3) | 0.0160(5) | 0.0206(4) |
| | $U_{33}$ | 0.0056(3) | 0.0064(3) | 0.0081(3) | 0.0117(3) | 0.0117(3) | 0.0157(4) | 0.0198(3) |
| | $U_{23}$ | -0.0007(2) | -0.0009(2) | -0.0008(2) | -0.0012(2) | -0.0012(2) | -0.0015(3) | -0.0022(2) |

**Table 15 Crystallographic details and refined parameters from joint refinement of "Anharmonic"-model against neutron and x-ray data of p-1BGS**

| p-1BGS "*Anharmonic model*" | | Joint neutron and x-ray | | | | |
|---|---|---|---|---|---|---|
| X-ray | Temperature | 100 | 200 | 300 | 300 | 400 |
| | $R_F$ | 4.08 | 4.3 | 4.86 | 4.81 | 5.99 |
| | $R_F(I_{obs}>3\sigma_{obs})$ | 2.84 | 2.4 | 2.33 | 2.29 | 2.46 |
| | $R_{wF}$ | 3.86 | 3 | 3.87 | 3.82 | 3.14 |
| | $R_{wF}(I_{obs}>3\sigma_{obs})$ | 3.17 | 2.68 | 2.52 | 2.46 | 2.69 |
| | Extinction | 0.044(10) | 0.035(8) | 0.109(10) | 0.111(10) | 0.116(9) |
| Neutron | $R_F$ | 6.35 | 6.52 | 5.74 | 7.84 | 6.27 |
| | $R_F(I_{obs}>3\sigma_{obs})$ | 4.13 | 4.35 | 3.61 | 4.92 | 3.94 |
| | $R_{wF}$ | 4.83 | 4.64 | 4.04 | 4.44 | 4.10 |
| | $R_{wF}(I_{obs}>3\sigma_{obs})$ | 4.69 | 4.49 | 3.88 | 4.20 | 3.82 |
| | Extinction | 0.001(3) | 0.028(3) | 0.023(3) | 0.028(3) | 0.029(3) |
| Ba(1) 2a | $U_{11}$ | 0.0112(1) | 0.0163(1) | 0.0216(2) | 0.0216(2) | 0.0277(2) |
| Ba(2) 6d | $U_{11}$ | 0.0222(8) | 0.0286(8) | 0.0350(10) | 0.0352(10) | 0.043(1) |
| | $U_{22}$ | 0.1307(8) | 0.1378(9) | 0.145(1) | 0.144(1) | 0.156(1) |
| | $C_{122}$ | 0.0069(2) | 0.0060(2) | 0.0056(3) | 0.0056(3) | 0.0055(2) |
| | $D_{1111}$ | 0.00016(7) | 0.00009(8) | 0.0000(1) | 0.0000(1) | 0.0000(1) |
| | $D_{1122}$ | -0.00019(7) | -0.00016(7) | -0.00039(9) | -0.00036(9) | -0.00048(10) |
| | $D_{2222}$ | -0.0190(4) | -0.0158(4) | -0.0145(5) | -0.0145(5) | -0.0137(5) |
| | $D_{2233}$ | -0.0136(3) | -0.0103(3) | -0.0085(4) | -0.0086(4) | -0.0084(4) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.0416(8) | 0.0421(6) | 0.0423(7) | 0.0417(8) | 0.0398(6) |
| | $U_{11}$ | 0.082(1) | 0.0806(8) | 0.0817(9) | 0.082(1) | 0.0826(8) |
| | $U_{22}$ | 0.0126(3) | 0.0156(3) | 0.0201(3) | 0.0203(3) | 0.0244(3) |
| | ai[Sn2] | 0.0121(2) | 0.0150(2) | 0.0191(2) | 0.0191(2) | 0.0232(2) |
| Sn/Ga(2) 16i | x | 0.2158(9) | 0.2162(7) | 0.2157(8) | 0.2142(9) | 0.2162(7) |
| | $U_{11}$ | 0.18406(2) | 0.18408(2) | 0.18410(2) | 0.18413(2) | 0.18411(2) |
| | $U_{12}$ | 0.01059(8) | 0.01425(8) | 0.01832(9) | 0.01832(10) | 0.02332(9) |
| | y | -0.00018(6) | -0.00047(5) | -0.00082(7) | -0.00079(7) | -0.00109(6) |
| Sn/Ga(3) 24k | z | 0.31234(2) | 0.31225(2) | 0.31221(2) | 0.31225(3) | 0.31223(2) |
| | $U_{11}$ | 0.11835(2) | 0.11834(2) | 0.11835(2) | 0.11839(2) | 0.11843(2) |
| | $U_{22}$ | 0.0128(1) | 0.0165(1) | 0.0209(1) | 0.0210(1) | 0.0265(1) |
| | $U_{33}$ | 0.0101(1) | 0.01367(10) | 0.0174(1) | 0.0174(1) | 0.0220(1) |
| | $U_{23}$ | 0.0098(1) | 0.01304(10) | 0.0168(1) | 0.0168(1) | 0.0213(1) |
| | ai[Sn1] | -0.00088(7) | -0.00116(7) | -0.00149(9) | -0.00148(9) | -0.00191(9) |

**Table 16 Crystallographic details and refined parameters from joint refinement of "Anharmonic"-model against neutron and x-ray data of n-1BGS**

| n-1BGS "*Anharmonic model*" | | Joint neutron and x-ray | | | |
|---|---|---|---|---|---|
| X-ray | Temperature | 100 | 200 | 300 | 400 |
| | $R_F$ | 3.62 | 3.86 | 4.52 | 5.3 |
| | $R_F(I_{obs}>3\sigma_{obs})$ | 2.47 | 2.27 | 2.12 | 2.27 |
| | $R_{wF}$ | 3.34 | 4.01 | 2.86 | 2.94 |
| | $R_{wF}(I_{obs}>3\sigma_{obs})$ | 3.19 | 2.67 | 2.54 | 2.55 |
| | Extinction | 0.042(7) | 0.047(8) | 0.050(6) | 0.080(7) |
| Neutron | $R_F$ | 6.84 | 7.54 | 6.36 | 5.77 |
| | $R_F(I_{obs}>3\sigma_{obs})$ | 4.29 | 4.21 | 3.78 | 3.24 |
| | $R_{wF}$ | 4.33 | 4.10 | 3.71 | 3.59 |
| | $R_{wF}(I_{obs}>3\sigma_{obs})$ | 4.09 | 3.75 | 3.33 | 3.37 |
| | Extinction | 0.024(3) | 0.022(3) | 0.020(2) | 0.020(2) |
| Ba(1) 2a | $U_{11}$ | 0.01014(9) | 0.0154(1) | 0.0211(1) | 0.0274(1) |
| Ba(2) 6d | $U_{11}$ | 0.0188(6) | 0.0263(8) | 0.0341(7) | 0.0429(8) |
| | $U_{22}$ | 0.1274(7) | 0.1326(9) | 0.1427(8) | 0.1543(9) |
| | $C_{122}$ | 0.0065(2) | 0.0057(2) | 0.0053(2) | 0.0055(2) |
| | $D_{1111}$ | 0.00005(5) | 0.00007(8) | 0.00004(8) | 0.0001(1) |
| | $D_{1122}$ | -0.00009(5) | -0.00014(7) | -0.00024(6) | -0.00043(8) |
| | $D_{2222}$ | -0.0183(3) | -0.0147(4) | -0.0140(3) | -0.0146(4) |
| | $D_{2233}$ | -0.0133(3) | -0.0095(3) | -0.0083(3) | -0.0075(3) |
| Sn/Ga(1) 6c | ai[Sn1] | 0.0349(7) | 0.0369(8) | 0.0357(6) | 0.0409(5) |
| | ai[Ga1] | 0.089(1) | 0.088(1) | 0.0889(9) | 0.0824(7) |
| | $U_{11}$ | 0.0113(2) | 0.0151(3) | 0.0191(2) | 0.0247(3) |
| | $U_{22}$ | 0.0102(1) | 0.0140(2) | 0.0179(2) | 0.0233(2) |
| Sn/Ga(2) 16i | ai[Sn2] | 0.2070(7) | 0.2074(7) | 0.2077(6) | 0.2138(5) |
| | X | 0.18424(1) | 0.18427(2) | 0.18427(1) | 0.18413(1) |
| | $U_{11}$ | 0.00953(6) | 0.01337(7) | 0.01793(6) | 0.02307(7) |
| | $U_{12}$ | 0.00002(4) | -0.00021(6) | -0.00056(5) | -0.00111(6) |
| Sn/Ga(3) 24k | Y | 0.31237(2) | 0.31232(2) | 0.31224(2) | 0.31225(2) |
| | Z | 0.11869(2) | 0.11873(2) | 0.11874(2) | 0.11849(2) |
| | $U_{11}$ | 0.01208(9) | 0.0161(1) | 0.02085(10) | 0.0263(1) |
| | $U_{22}$ | 0.00907(8) | 0.01261(10) | 0.01689(9) | 0.0218(1) |
| | $U_{33}$ | 0.00866(8) | 0.01196(10) | 0.01613(8) | 0.02100(10) |
| | $U_{23}$ | -0.00112(6) | -0.00130(7) | -0.00167(6) | -0.00182(7) |

## Refined parameters: 8BGS

**Table 17 Crystallographic details and refined parameters from refinement of "Anharmonic"-model against neutron data of n-8BGS.**

| n-8BGS "*Anharmonic model*" | | Radiation source: | | | Neutron | | | |
|---|---|---|---|---|---|---|---|---|
| Temperature | | 10 | 50 | 100 | 200 | 300 | 400 | 500 |
| $N_{par}$ | | 27 | 27 | 27 | 27 | 27 | 27 | 27 |
| $N_{obs}$ | | 318 | 318 | 318 | 321 | 327 | 292 | 280 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 303 | 304 | 298 | 287 | 283 | 284 | 261 |
| $R_F$ | | 2.3 | 2.45 | 2.9 | 3.45 | 4.47 | 2.16 | 2.56 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 1.99 | 2.13 | 2.26 | 2.32 | 3.01 | 1.96 | 1.97 |
| $R_{wF}$ | | 1.91 | 2.01 | 2.10 | 2.12 | 2.30 | 1.9 | 1.99 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 1.89 | 1.98 | 2.04 | 1.98 | 2.18 | 1.86 | 1.91 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.024(2) | 0.024(2) | 0.023(2) | 0.021(2) | 0.019(2) | 0.019(2) | 0.026(3) |
| Ba | x | 0.8152(2) | 0.8152(2) | 0.8150(2) | 0.8149(2) | 0.8149(2) | 0.8148(2) | 0.8146(2) |
| | $U_{11}$ | 0.0170(6) | 0.0187(6) | 0.0235(7) | 0.0311(8) | 0.040(1) | 0.0473(9) | 0.052(1) |
| | $U_{12}$ | -0.0002(1) | -0.0001(1) | -0.0002(1) | -0.0002(2) | 0.0000(2) | -0.0005(1) | -0.0005(2) |
| | $C_{111}$ | 0.0002(2) | 0.0001(2) | -0.0000(2) | 0.0000(2) | -0.0000(3) | -0.0004(2) | -0.0009(3) |
| | $C_{112}$ | -0.00021(6) | -0.00019(6) | -0.00019(7) | -0.00015(8) | -0.0002(1) | 0.00002(9) | -0.0000(1) |
| | $C_{123}$ | 0.00032(9) | 0.0004(1) | 0.0005(1) | 0.0004(2) | 0.0005(2) | 0.0003(2) | 0.0000(2) |
| | $D_{1111}$ | -0.00004(8) | -0.00012(9) | -0.0000(1) | -0.0002(1) | -0.0001(2) | -0.0003(1) | -0.0004(2) |
| | $D_{1112}$ | 0.00010(3) | 0.00010(4) | 0.00009(4) | 0.00015(5) | 0.00009(7) | 0.00022(5) | 0.00023(6) |
| | $D_{1122}$ | -0.00001(2) | 0.00000(2) | -0.00000(3) | -0.00001(3) | 0.00002(4) | 0.00002(4) | -0.00001(5) |
| | $D_{1123}$ | -0.0039(6) | -0.0044(7) | -0.0062(7) | -0.0076(8) | -0.0098(9) | -0.0103(8) | -0.0116(9) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.201(7) | 0.193(6) | 0.192(7) | 0.191(7) | 0.193(7) | 0.203(6) | 0.203(6) |
| | $U_{11}$ | 0.0069(3) | 0.0071(3) | 0.0090(4) | 0.0124(4) | 0.0154(5) | 0.0192(3) | 0.0217(4) |
| | $U_{22}$ | 0.0110(3) | 0.0122(3) | 0.0139(3) | 0.0187(3) | 0.0236(4) | 0.0282(3) | 0.0313(4) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.031(2) | 0.033(2) | 0.033(3) | 0.032(3) | 0.035(3) | 0.036(2) | 0.036(2) |
| | $U_{11}$ | 0.0050(4) | 0.0050(4) | 0.0064(4) | 0.0094(5) | 0.0117(5) | 0.0152(4) | 0.0173(5) |
| Sn/Ga(3) 24g | ai[Sn3] | 0.352(8) | 0.354(8) | 0.353(9) | 0.364(9) | 0.358(9) | 0.345(8) | 0.354(8) |
| | x | 0.58432(3) | 0.58432(3) | 0.58432(4) | 0.58432(4) | 0.58429(4) | 0.58430(3) | 0.58438(4) |
| | z | 0.85084(4) | 0.85082(4) | 0.85083(5) | 0.85091(5) | 0.85087(5) | 0.85098(4) | 0.85061(5) |
| | $U_{11}$ | 0.0058(1) | 0.0067(2) | 0.0084(2) | 0.0123(2) | 0.0171(2) | 0.0220(2) | 0.0252(2) |
| | $U_{33}$ | 0.0060(2) | 0.0064(2) | 0.0076(2) | 0.0107(3) | 0.0138(3) | 0.0180(2) | 0.0198(3) |
| | $U_{12}$ | -0.0001(1) | 0.0001(1) | -0.0002(2) | -0.0002(2) | -0.0005(2) | -0.0008(2) | -0.0007(2) |
| | $U_{13}$ | -0.00001(9) | 0.00003(9) | 0.0001(1) | 0.0001(1) | 0.0000(1) | 0.0001(1) | 0.0002(1) |
| Sn/Ga(3) 8c | x | 0.63423(4) | 0.63424(4) | 0.63424(4) | 0.63421(4) | 0.63418(5) | 0.63415(4) | 0.63419(4) |
| | $U_{11}$ | 0.0051(2) | 0.0055(2) | 0.0068(2) | 0.0103(2) | 0.0136(3) | 0.0175(2) | 0.0201(2) |
| | $U_{12}$ | -0.0002(1) | -0.0001(1) | -0.0002(1) | -0.0002(2) | 0.0000(2) | -0.0005(1) | -0.0005(2) |

**Table 18 Crystallographic details and refined parameters from refinement of "Anharmonic"-model against neutron data of p-8BGS**

| p-8BGS *"Anharmonic model"* | | Radiation source: | | Neutron | | |
|---|---|---|---|---|---|---|
| Temperature | | 10 | 50 | 100 | 200 | 300 |
| $N_{par}$ | | 27 | 27 | 27 | 27 | 27 |
| $N_{obs}$ | | 436 | 440 | 436 | 439 | 437 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 361 | 367 | 359 | 323 | 292 |
| $R_F$ | | 5.33 | 5.95 | 6.95 | 8.75 | 10.98 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 2.89 | 3.56 | 3.95 | 3.67 | 3.68 |
| $R_{wF}$ | | 2.07 | 2.26 | 2.53 | 2.61 | 2.76 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 1.85 | 2.14 | 2.36 | 2.26 | 2.22 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.018(1) | 0.019(2) | 0.027(2) | 0.031(2) | 0.030(2) |
| Ba | x | 0.8153(1) | 0.8152(2) | 0.8150(2) | 0.8149(2) | 0.8143(2) |
| | $U_{11}$ | 0.0147(6) | 0.0181(7) | 0.0225(8) | 0.0296(9) | 0.040(1) |
| | $U_{12}$ | -0.0001(1) | 0.0000(1) | 0.0001(2) | -0.0001(2) | 0.0002(2) |
| | $C_{111}$ | -0.0000(1) | -0.0001(2) | -0.0002(2) | -0.0005(2) | -0.0011(3) |
| | $C_{112}$ | -0.00003(5) | -0.00013(6) | -0.00012(7) | -0.00003(9) | -0.0001(1) |
| | $C_{123}$ | 0.00014(9) | 0.0000(1) | 0.0002(1) | 0.0002(2) | 0.0000(3) |
| | $D_{1111}$ | -0.00011(7) | -0.00015(9) | -0.0002(1) | -0.0003(1) | -0.0001(2) |
| | $D_{1112}$ | 0.00008(3) | 0.00013(4) | 0.00005(4) | 0.00016(5) | 0.00021(8) |
| | $D_{1122}$ | 0.00001(2) | -0.00003(2) | 0.00004(3) | 0.00006(4) | -0.00001(6) |
| | $D_{1123}$ | -0.0042(6) | -0.0046(7) | -0.0062(8) | -0.0067(9) | -0.009(1) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.196(6) | 0.196(6) | 0.196(7) | 0.199(7) | 0.209(7) |
| | $U_{11}$ | 0.0061(3) | 0.0069(3) | 0.0089(4) | 0.0117(4) | 0.0155(5) |
| | $U_{22}$ | 0.0108(2) | 0.0118(3) | 0.0140(3) | 0.0185(4) | 0.0226(4) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.029(2) | 0.030(2) | 0.031(3) | 0.030(3) | 0.029(3) |
| | $U_{11}$ | 0.0049(4) | 0.0051(4) | 0.0069(5) | 0.0095(5) | 0.0134(6) |
| Sn/Ga(3) 24g | ai[Sn3] | 0.344(8) | 0.346(9) | 0.342(9) | 0.341(9) | 0.340(10) |
| | x | 0.58417(3) | 0.58417(3) | 0.58418(4) | 0.58419(4) | 0.58415(5) |
| | z | 0.85112(4) | 0.85114(4) | 0.85121(5) | 0.85120(5) | 0.85125(6) |
| | $U_{11}$ | 0.0054(1) | 0.0064(1) | 0.0089(2) | 0.0128(2) | 0.0175(2) |
| | $U_{33}$ | 0.0054(2) | 0.0059(2) | 0.0082(2) | 0.0109(3) | 0.0140(3) |
| | $U_{12}$ | 0.0000(1) | 0.0000(2) | 0.0000(2) | -0.0003(2) | -0.0002(3) |
| | $U_{13}$ | -0.00023(9) | -0.0002(1) | -0.0001(1) | -0.0000(1) | 0.0002(2) |
| Sn/Ga(3) 8c | x | 0.63422(4) | 0.63417(4) | 0.63411(4) | 0.63412(5) | 0.63411(5) |
| | $U_{11}$ | 0.0046(2) | 0.0054(2) | 0.0071(2) | 0.0101(3) | 0.0142(3) |
| | $U_{12}$ | -0.0001(1) | 0.0000(1) | 0.0001(2) | -0.0001(2) | 0.0002(2) |

**Table 19 Crystallographic details and refined parameters from refinement of "Anharmonic"-model against x-ray data of n-8BGS**

| n-8BGS "*Anharmonic model*" | | Radiation source: | | X-ray | | |
|---|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 300 | 400 |
| $N_{par}$ | | 27 | 27 | 27 | 27 | 27 |
| $N_{obs}$ | | 2460 | 2359 | 2004 | 1914 | 2149 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 2108 | 1529 | 1322 | 1466 | 1163 |
| $R_F$ | | 3.67 | 2.56 | 4.56 | 4.09 | 6.63 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 2.82 | 2.56 | 2.59 | 2.8 | 2.61 |
| $R_{wF}$ | | 3.16 | 2.4 | 3.39 | 3.43 | 3.27 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 3.02 | 2.4 | 2.63 | 3.05 | 2.6 |
| $R_{internal}$ | | 4.09 | 3.25 | 2.9 | 3.19 | 2.58 |
| extinction | | 0.069(4) | 0.068(3) | 0.066(3) | 0.040(4) | 0.070(4) |
| Ba | x | 0.81507(4) | 0.81477(5) | 0.81464(6) | 0.81462(7) | 0.81443(6) |
| | $U_{11}$ | 0.0255(2) | 0.0345(2) | 0.0430(3) | 0.0413(3) | 0.0496(3) |
| | $U_{12}$ | -0.00017(6) | -0.00002(8) | -0.00016(10) | -0.00009(8) | -0.00023(9) |
| | $C_{111}$ | -0.00022(4) | -0.00048(5) | -0.00068(8) | -0.00072(8) | -0.0009(1) |
| | $C_{112}$ | -0.00005(1) | -0.00006(2) | -0.00001(3) | -0.00002(3) | -0.00003(3) |
| | $C_{123}$ | 0.00018(3) | 0.00019(4) | 0.00029(7) | 0.00025(6) | 0.00036(7) |
| | $D_{1111}$ | -0.00010(1) | -0.00010(3) | -0.00010(4) | -0.00017(4) | -0.00011(6) |
| | $D_{1112}$ | 0.000043(6) | 0.00010(1) | 0.00010(2) | 0.00012(1) | 0.00015(2) |
| | $D_{1122}$ | -0.000009(4) | -0.000001(7) | 0.00002(1) | 0.000002(9) | 0.00001(1) |
| | $D_{1123}$ | -0.0070(1) | -0.0082(2) | -0.0102(3) | -0.0099(3) | -0.0120(2) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.202(1) | 0.2020(9) | 0.203(1) | 0.206(1) | 0.202(1) |
| | $U_{11}$ | 0.01007(10) | 0.0131(1) | 0.0170(1) | 0.0155(1) | 0.0185(2) |
| | $U_{22}$ | 0.01584(9) | 0.0198(1) | 0.0250(1) | 0.0235(1) | 0.0279(1) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.0347(4) | 0.0353(4) | 0.0352(4) | 0.0332(5) | 0.0346(4) |
| | $U_{11}$ | 0.0075(1) | 0.0104(1) | 0.0136(2) | 0.0113(1) | 0.0146(2) |
| Sn/Ga(3) 24g | ai[Sn3] | 0.340(1) | 0.339(1) | 0.339(1) | 0.340(1) | 0.340(1) |
| | x | 0.58453(1) | 0.58448(2) | 0.58449(2) | 0.58450(2) | 0.58449(2) |
| | z | 0.85106(2) | 0.85110(2) | 0.85113(3) | 0.85113(2) | 0.85121(2) |
| | $U_{11}$ | 0.01041(5) | 0.01440(7) | 0.01896(8) | 0.01750(7) | 0.02184(9) |
| | $U_{33}$ | 0.00866(6) | 0.01158(8) | 0.01500(10) | 0.01336(10) | 0.0165(1) |
| | $U_{12}$ | -0.00037(5) | -0.00065(7) | -0.00083(10) | -0.00073(8) | -0.00095(9) |
| | $U_{13}$ | 0.00012(3) | 0.00006(4) | 0.00006(6) | 0.00017(5) | 0.00023(5) |
| Sn/Ga(3) 8c | x | 0.63426(2) | 0.63426(2) | 0.63420(3) | 0.63424(3) | 0.63419(3) |
| | $U_{11}$ | 0.00870(8) | 0.0120(1) | 0.0154(1) | 0.0136(1) | 0.0173(1) |
| | $U_{12}$ | -0.00017(6) | -0.00002(8) | -0.00016(10) | -0.00009(8) | -0.00023(9) |

**Table 20 Crystallographic details and refined parameters from refinement of "Anharmonic"-model against x-ray data of p-8BGS**

| p-8BGS "*Anharmonic model*" | | Radiation source: X-ray | | | |
|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 400 |
| $N_{par}$ | | 27 | 27 | 27 | 27 |
| $N_{obs}$ | | 1321 | 1333 | 1333 | 1335 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 1270 | 1290 | 1170 | 1086 |
| $R_F$ | | 1.88 | 1.84 | 2.26 | 2.7 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 1.76 | 1.74 | 1.8 | 1.9 |
| $R_{wF}$ | | 2.29 | 2.41 | 2.1 | 2.18 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 2.27 | 2.39 | 1.99 | 2.04 |
| $R_{internal}$ | | 2.87 | 5.33 | 2.95 | 3.11 |
| extinction | | 0.052(5) | 0.068(5) | 0.142(5) | 0.143(6) |
| Ba | x | 0.81509(4) | 0.81501(4) | 0.81466(5) | 0.81455(5) |
| | $U_{11}$ | 0.0264(2) | 0.0305(2) | 0.0438(2) | 0.0520(3) |
| | $U_{12}$ | 0.00002(6) | 0.00002(6) | -0.00004(7) | 0.00006(8) |
| | $C_{111}$ | -0.00018(4) | -0.00024(4) | -0.00066(6) | -0.00083(7) |
| | $C_{112}$ | -0.00006(1) | -0.00006(1) | -0.00001(2) | 0.00001(2) |
| | $C_{123}$ | 0.00015(3) | 0.00018(3) | 0.00023(4) | 0.00032(6) |
| | $D_{1111}$ | -0.00004(2) | -0.00003(2) | -0.00008(3) | -0.00020(4) |
| | $D_{1112}$ | 0.000056(6) | 0.000061(7) | 0.00010(1) | 0.00016(1) |
| | $D_{1122}$ | 0.000002(4) | 0.000008(5) | 0.000013(7) | 0.000003(9) |
| | $D_{1123}$ | -0.0065(2) | -0.0073(2) | -0.0102(2) | -0.0117(2) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.208(1) | 0.208(1) | 0.207(1) | 0.205(1) |
| | $U_{11}$ | 0.0115(1) | 0.0130(1) | 0.0180(1) | 0.0214(1) |
| | $U_{22}$ | 0.01713(10) | 0.0191(1) | 0.0260(1) | 0.0307(1) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.0315(5) | 0.0317(5) | 0.0325(4) | 0.0326(5) |
| | $U_{11}$ | 0.0084(2) | 0.0099(2) | 0.0146(2) | 0.0180(2) |
| Sn/Ga(3) 24g | ai[Sn3] | 0.336(2) | 0.336(2) | 0.334(1) | 0.335(2) |
| | x | 0.58439(1) | 0.58439(1) | 0.58433(1) | 0.58430(2) |
| | z | 0.85135(2) | 0.85138(2) | 0.85142(2) | 0.85144(2) |
| | $U_{11}$ | 0.01148(6) | 0.01342(6) | 0.01995(7) | 0.02466(8) |
| | $U_{33}$ | 0.00984(8) | 0.01119(8) | 0.01624(8) | 0.01974(10) |
| | $U_{12}$ | -0.00014(5) | -0.00026(5) | -0.00052(6) | -0.00070(7) |
| | $U_{13}$ | 0.00005(4) | 0.00003(4) | 0.00003(4) | 0.00015(5) |
| Sn/Ga(3) 8c | x | 0.63426(2) | 0.63424(2) | 0.63425(2) | 0.63421(2) |
| | $U_{11}$ | 0.0094(1) | 0.0109(1) | 0.0163(1) | 0.0201(1) |
| | $U_{12}$ | 0.00002(6) | 0.00002(6) | -0.00004(7) | 0.00006(8) |

**Table 21 Crystallographic details and refined parameters from refinement of "Harmonic"-model against neutron data of n-8BGS**

| n-8BGS *"Harmonic model"* | | Radiation source: Neutron | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Temperature | | 10 | 50 | 100 | 200 | 300 | 400 | 500 |
| $N_{par}$ | | 20 | 20 | 20 | 20 | 20 | 20 | 20 |
| $N_{obs}$ | | 318 | 318 | 318 | 321 | 327 | 292 | 280 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 303 | 304 | 298 | 287 | 283 | 284 | 261 |
| $R_F$ | | 2.31 | 2.51 | 2.93 | 3.49 | 4.49 | 2.24 | 2.66 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 2.02 | 2.18 | 2.28 | 2.34 | 3.05 | 2.04 | 2.05 |
| $R_{wF}$ | | 2.02 | 2.11 | 2.18 | 2.19 | 2.34 | 2.02 | 2.11 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 1.99 | 2.07 | 2.12 | 2.05 | 2.23 | 1.98 | 2.03 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.025(2) | 0.025(2) | 0.023(2) | 0.021(2) | 0.019(2) | 0.019(2) | 0.026(3) |
| Ba 8c | x | 0.81537(7) | 0.81535(7) | 0.81524(8) | 0.81506(9) | 0.81510(10) | 0.81497(9) | 0.81505(10) |
| | $U_{11}$ | 0.0174(3) | 0.0200(3) | 0.0243(3) | 0.0332(4) | 0.0414(5) | 0.0505(4) | 0.0553(5) |
| | $U_{12}$ | -0.0056(2) | -0.0062(3) | -0.0075(3) | -0.0096(3) | -0.0109(4) | -0.0128(4) | -0.0137(4) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.197(7) | 0.189(7) | 0.189(7) | 0.188(7) | 0.191(7) | 0.202(6) | 0.204(6) |
| | $U_{11}$ | 0.0070(3) | 0.0073(4) | 0.0091(4) | 0.0126(4) | 0.0155(5) | 0.0193(4) | 0.0217(4) |
| | $U_{22}$ | 0.0110(3) | 0.0122(3) | 0.0140(3) | 0.0187(3) | 0.0236(4) | 0.0281(3) | 0.0311(4) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.032(3) | 0.034(3) | 0.033(3) | 0.033(3) | 0.035(3) | 0.036(2) | 0.036(2) |
| | $U_{11}$ | 0.0048(4) | 0.0049(4) | 0.0063(4) | 0.0092(5) | 0.0117(5) | 0.0152(4) | 0.0172(5) |
| Sn/Ga(3) 24g | ai[Sn3] | 0.353(9) | 0.356(9) | 0.355(9) | 0.366(9) | 0.360(9) | 0.348(8) | 0.356(8) |
| | x | 0.58431(3) | 0.58430(3) | 0.58431(4) | 0.58430(4) | 0.58428(4) | 0.58426(3) | 0.58436(4) |
| | z | 0.85088(4) | 0.85085(4) | 0.85086(5) | 0.85094(5) | 0.85089(5) | 0.85100(4) | 0.85063(5) |
| | $U_{11}$ | 0.0057(1) | 0.0067(2) | 0.0084(2) | 0.0123(2) | 0.0171(2) | 0.0221(2) | 0.0252(2) |
| | $U_{33}$ | 0.0060(2) | 0.0064(2) | 0.0076(2) | 0.0107(3) | 0.0137(3) | 0.0179(2) | 0.0197(3) |
| | $U_{12}$ | -0.0001(1) | 0.0001(2) | -0.0003(2) | -0.0002(2) | -0.0005(2) | -0.0008(2) | -0.0007(2) |
| | $U_{13}$ | -0.00001(9) | 0.00004(10) | 0.0001(1) | 0.0001(1) | 0.0001(1) | 0.0002(1) | 0.0002(1) |
| Sn/Ga (3) 8c | x | 0.63423(4) | 0.63425(4) | 0.63425(4) | 0.63422(4) | 0.63418(5) | 0.63416(4) | 0.63420(4) |
| | $U_{11}$ | 0.0050(2) | 0.0055(2) | 0.0067(2) | 0.0103(2) | 0.0136(3) | 0.0176(2) | 0.0202(2) |
| | $U_{12}$ | -0.0002(1) | -0.0001(1) | -0.0002(1) | -0.0002(2) | 0.0000(2) | -0.0005(1) | -0.0005(2) |

**Table 22 Crystallographic details and refined parameters from refinement of "Harmonic"-model against neutron data of p-8BGS**

| p-8BGS *"Harmonic model"* | | Radiation source: | | Neutron | | |
|---|---|---|---|---|---|---|
| Temperature | | 10 | 50 | 100 | 200 | 300 |
| $N_{par}$ | | 20 | 20 | 20 | 20 | 20 |
| $N_{obs}$ | | 436 | 440 | 436 | 439 | 437 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 361 | 367 | 359 | 323 | 292 |
| $R_F$ | | 5.39 | 5.95 | 6.9 | 8.87 | 10.98 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 2.94 | 3.59 | 3.96 | 3.79 | 3.72 |
| $R_{wF}$ | | 2.11 | 2.31 | 2.57 | 2.69 | 2.83 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 1.89 | 2.19 | 2.4 | 2.36 | 2.32 |
| $R_{internal}$ | | 0 | 0 | 0 | 0 | 0 |
| extinction | | 0.018(1) | 0.019(2) | 0.027(2) | 0.030(2) | 0.030(2) |
| Ba 8c | x | 0.81532(6) | 0.81538(7) | 0.81531(8) | 0.81525(10) | 0.8151(1) |
| | $U_{11}$ | 0.0163(2) | 0.0191(3) | 0.0242(3) | 0.0327(4) | 0.0413(5) |
| | $U_{12}$ | -0.0056(2) | -0.0064(3) | -0.0074(3) | -0.0094(4) | -0.0108(5) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.195(6) | 0.194(7) | 0.195(7) | 0.198(7) | 0.207(7) |
| | $U_{11}$ | 0.0062(3) | 0.0070(3) | 0.0090(4) | 0.0119(4) | 0.0155(5) |
| | $U_{22}$ | 0.0108(2) | 0.0118(3) | 0.0141(3) | 0.0184(4) | 0.0226(4) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.029(2) | 0.030(2) | 0.031(3) | 0.031(3) | 0.029(3) |
| | $U_{11}$ | 0.0048(4) | 0.0049(4) | 0.0069(5) | 0.0094(5) | 0.0131(6) |
| Sn/Ga(3) 24g | ai[Sn3] | 0.344(8) | 0.347(9) | 0.343(9) | 0.342(9) | 0.34(1) |
| | x | 0.58416(3) | 0.58417(3) | 0.58416(4) | 0.58418(4) | 0.58415(5) |
| | z | 0.85113(4) | 0.85117(4) | 0.85122(5) | 0.85121(5) | 0.85127(6) |
| | $U_{11}$ | 0.0055(1) | 0.0064(1) | 0.0089(2) | 0.0129(2) | 0.0174(2) |
| | $U_{33}$ | 0.0054(2) | 0.0059(2) | 0.0081(3) | 0.0108(3) | 0.0139(3) |
| | $U_{12}$ | -0.0000(1) | -0.0000(2) | -0.0000(2) | -0.0004(2) | -0.0003(3) |
| | $U_{13}$ | -0.00023(9) | -0.0002(1) | -0.0001(1) | -0.0000(1) | 0.0002(2) |
| Sn/Ga(3) 8c | x | 0.63422(4) | 0.63416(4) | 0.63411(4) | 0.63411(5) | 0.63410(5) |
| | $U_{11}$ | 0.0046(2) | 0.0054(2) | 0.0072(2) | 0.0102(3) | 0.0141(3) |
| | $U_{12}$ | -0.0001(1) | 0.0001(1) | 0.0001(2) | -0.0001(2) | 0.0003(2) |

**Table 23 Crystallographic details and refined parameters from refinement of "Harmonic"-model against x-ray data of n-8BGS**

| n-8BGS *"Harmonic model"* | | Radiation source: | | X-ray | | |
|---|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 300 | 400 |
| $N_{par}$ | | 20 | 20 | 20 | 20 | 20 |
| $N_{obs}$ | | 2460 | 2359 | 2004 | 1914 | 2149 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 2108 | 1529 | 1322 | 1466 | 1163 |
| $R_F$ | | 3.76 | 5.87 | 4.7 | 4.23 | 6.79 |
| $R_F(I_{obs}>3\sigma_{obs})$ | | 2.91 | 2.66 | 2.7 | 2.95 | 2.77 |
| $R_{wF}$ | | 3.26 | 3.04 | 3.52 | 3.6 | 3.42 |
| $R_{wF}(I_{obs}>3\sigma_{obs})$ | | 3.12 | 2.56 | 2.76 | 3.23 | 2.78 |
| $R_{internal}$ | | 4.09 | 3.25 | 2.9 | 3.19 | 2.58 |
| extinction | | 0.070(4) | 0.071(3) | 0.066(4) | 0.039(4) | 0.071(4) |
| Ba 8c | x | 0.81535(2) | 0.81515(2) | 0.81504(3) | 0.81513(4) | 0.81487(3) |
| | $U_{11}$ | 0.02668(9) | 0.0355(1) | 0.0445(2) | 0.0434(2) | 0.0519(2) |
| | $U_{12}$ | -0.00770(7) | -0.00962(9) | -0.0114(1) | -0.0115(1) | -0.0133(1) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.203(1) | 0.2018(9) | 0.203(1) | 0.205(1) | 0.202(1) |
| | $U_{11}$ | 0.0101(1) | 0.0132(1) | 0.0169(2) | 0.0155(2) | 0.0186(2) |
| | $U_{22}$ | 0.01589(9) | 0.0199(1) | 0.0250(1) | 0.0235(1) | 0.0278(1) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.0348(4) | 0.0353(4) | 0.0354(4) | 0.0335(6) | 0.0350(4) |
| | $U_{11}$ | 0.0075(1) | 0.0105(1) | 0.0137(2) | 0.0113(2) | 0.0148(2) |
| Sn/Ga(3) 24g | ai[Sn3] | 0.340(1) | 0.340(1) | 0.340(1) | 0.341(1) | 0.341(1) |
| | x | 0.58452(1) | 0.58447(2) | 0.58447(2) | 0.58448(2) | 0.58448(2) |
| | z | 0.85106(2) | 0.85110(2) | 0.85112(3) | 0.85112(3) | 0.85121(2) |
| | $U_{11}$ | 0.01047(5) | 0.01456(6) | 0.01902(8) | 0.01756(8) | 0.02201(10) |
| | $U_{33}$ | 0.00871(7) | 0.01168(8) | 0.01510(10) | 0.0134(1) | 0.0165(1) |
| | $U_{12}$ | -0.00036(6) | -0.00063(7) | -0.00083(10) | -0.00075(8) | -0.00091(9) |
| | $U_{13}$ | 0.00012(4) | 0.00007(4) | 0.00006(6) | 0.00019(5) | 0.00020(6) |
| Sn/Ga(3) 8c | x | 0.63428(2) | 0.63425(2) | 0.63422(3) | 0.63425(3) | 0.63421(3) |
| | $U_{11}$ | 0.00866(8) | 0.01193(10) | 0.0153(1) | 0.0136(1) | 0.0173(1) |
| | $U_{12}$ | -0.00016(6) | -0.00002(8) | -0.0002(1) | -0.00009(8) | -0.00023(10) |

**Table 24 Crystallographic details and refined parameters from refinement of "Harmonic"-model against x-ray data of p-8BGS**

| p-8BGS "*Harmonic model*" | | Radiation source: | | X-ray | |
|---|---|---|---|---|---|
| Temperature | | 100 | 200 | 300 | 400 |
| $N_{par}$ | | 20 | 20 | 20 | 20 |
| $N_{obs}$ | | 1321 | 1333 | 1333 | 1335 |
| $N_{obs}$ ($I_{obs}>3\sigma_{obs}$) | | 1270 | 1290 | 1170 | 1086 |
| $R_F$ | | 1.96 | 1.95 | 2.45 | 2.95 |
| $R_F$($I_{obs}>3\sigma_{obs}$) | | 1.84 | 1.85 | 1.99 | 2.13 |
| $R_{wF}$ | | 2.43 | 2.56 | 2.34 | 2.46 |
| $R_{wF}$($I_{obs}>3\sigma_{obs}$) | | 2.41 | 2.54 | 2.24 | 2.34 |
| $R_{internal}$ | | 2.87 | 5.33 | 2.95 | 3.11 |
| extinction | | 0.052(5) | 0.069(6) | 0.143(6) | 0.144(6) |
| Ba 8c | x | 0.81535(2) | 0.81529(2) | 0.81509(2) | 0.81500(3) |
| | $U_{11}$ | 0.02728(9) | 0.03145(10) | 0.0456(1) | 0.0545(2) |
| | $U_{12}$ | -0.00750(7) | -0.00842(7) | -0.01147(10) | -0.0133(1) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.209(1) | 0.208(1) | 0.206(1) | 0.205(1) |
| | $U_{11}$ | 0.0116(1) | 0.0130(1) | 0.0181(1) | 0.0215(2) |
| | $U_{22}$ | 0.0171(1) | 0.0192(1) | 0.0260(1) | 0.0308(1) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.0315(5) | 0.0316(5) | 0.0328(5) | 0.0330(5) |
| | $U_{11}$ | 0.0084(2) | 0.0098(2) | 0.0147(2) | 0.0181(2) |
| Sn/Ga(3) 24g | ai[Sn3] | 0.336(2) | 0.336(2) | 0.334(2) | 0.335(2) |
| | x | 0.58438(1) | 0.58437(1) | 0.58431(2) | 0.58427(2) |
| | z | 0.85136(2) | 0.85139(2) | 0.85142(2) | 0.85145(2) |
| | $U_{11}$ | 0.01152(6) | 0.01346(6) | 0.02001(7) | 0.02474(9) |
| | $U_{33}$ | 0.00987(8) | 0.01121(8) | 0.01626(9) | 0.0198(1) |
| | $U_{12}$ | -0.00015(6) | -0.00026(6) | -0.00054(7) | -0.00070(8) |
| | $U_{13}$ | 0.00004(4) | 0.00003(4) | 0.00004(4) | 0.00014(5) |
| Sn/Ga(3) 8c | x | 0.63427(2) | 0.63425(2) | 0.63425(2) | 0.63422(2) |
| | $U_{11}$ | 0.0094(1) | 0.0108(1) | 0.0164(1) | 0.0201(1) |
| | $U_{12}$ | 0.00004(6) | 0.00004(6) | -0.00006(7) | 0.00003(8) |

**Table 25 Crystallographic details and refined parameters from joint refinement of "Harmonic"-model against neutron and x-ray data of n-8BGS**

| n-8BGS *"Harmonic model"* | | Joint neutron and x-ray refinement | | | | |
|---|---|---|---|---|---|---|
| X-ray | Temperature | 100 | 200 | 300 | 300 | 400 |
| | $R_F$ | 3.75 | 4.35 | 4.78 | 4.24 | 6.82 |
| | $R_F(I_{obs}>3\sigma_{obs})$ | 2.86 | 3.29 | 2.76 | 2.97 | 2.83 |
| | $R_{wF}$ | 3.24 | 2.88 | 3.57 | 3.61 | 3.47 |
| | $R_{wF}(I_{obs}>3\sigma_{obs})$ | 3.09 | 2.78 | 2.82 | 3.25 | 2.83 |
| | Extinction | 0.067(4) | 0.063(3) | 0.058(4) | 0.039(4) | 0.074(4) |
| Neutron | $R_F$ | 3.99 | 5.29 | 5.12 | 4.65 | 2.41 |
| | $R_F(I_{obs}>3\sigma_{obs})$ | 3.37 | 2.65 | 3.71 | 3.18 | 2.21 |
| | $R_{wF}$ | 3.1 | 2.89 | 2.91 | 2.51 | 2.23 |
| | $R_{wF}(I_{obs}>3\sigma_{obs})$ | 3.06 | 2.53 | 2.82 | 2.4 | 2.2 |
| | Extinction | 0.038(3) | 0.033(2) | 0.034(2) | 0.020(2) | 0.016(2) |
| Ba 8c | x | 0.81534(2) | 0.81515(2) | 0.81504(3) | 0.81513(3) | 0.81490(3) |
| | $U_{11}$ | 0.02649(10) | 0.03534(10) | 0.0441(2) | 0.0432(2) | 0.0521(2) |
| | $U_{12}$ | -0.00766(7) | -0.00963(8) | -0.0113(1) | -0.0114(1) | -0.0133(1) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.201(1) | 0.2012(4) | 0.2014(10) | 0.202(1) | 0.2005(8) |
| | $U_{11}$ | 0.00990(10) | 0.0130(1) | 0.0167(1) | 0.0154(1) | 0.0189(2) |
| | $U_{22}$ | 0.01563(8) | 0.01971(8) | 0.0248(1) | 0.0234(1) | 0.0281(1) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.0346(4) | 0.0349(2) | 0.0349(4) | 0.0340(5) | 0.0349(3) |
| | $U_{11}$ | 0.0073(1) | 0.01018(10) | 0.0134(1) | 0.0116(1) | 0.0150(1) |
| Sn/Ga(3) 24g | ai[Ga3] | 0.343(1) | 0.3415(4) | 0.343(1) | 0.344(1) | 0.3432(9) |
| | ai[Sn3] | 0.155(2) | 0.1561(8) | 0.153(2) | 0.151(2) | 0.153(1) |
| | x | 0.58449(1) | 0.58444(1) | 0.58441(2) | 0.58443(2) | 0.58441(2) |
| | z | 0.85103(2) | 0.85107(2) | 0.85106(2) | 0.85106(2) | 0.85112(2) |
| | $U_{11}$ | 0.01026(5) | 0.01420(5) | 0.01871(8) | 0.01748(7) | 0.02200(8) |
| | $U_{33}$ | 0.00858(7) | 0.01151(7) | 0.01497(10) | 0.01345(10) | 0.0171(1) |
| | $U_{12}$ | -0.00033(5) | -0.00053(6) | -0.00071(9) | -0.00069(8) | -0.00089(8) |
| | $U_{13}$ | 0.00011(3) | 0.00008(4) | 0.00007(6) | 0.00018(5) | 0.00021(5) |
| Sn/Ga(3) 8c | X | 0.63427(2) | 0.63424(2) | 0.63420(3) | 0.63421(2) | 0.63418(2) |
| | $U_{11}$ | 0.00836(8) | 0.01150(8) | 0.0149(1) | 0.0136(1) | 0.0175(1) |
| | $U_{12}$ | -0.00018(6) | -0.00009(6) | -0.00016(9) | -0.00008(7) | -0.00039(8) |

**Table 26 Crystallographic details and refined parameters from joint refinement of "Harmonic"-model against neutron and x-ray data of n-8BGS**

p-8BGS *"Harmonic model"* Joint neutron and x-ray refinement

| | | | | |
|---|---|---|---|---|
| X-ray | Temperature | 100 | 200 | 300 |
| | $R_F$ | 8.4 | 10.5 | 12.28 |
| | $R_F(I_{obs}>3\sigma_{obs})$ | 5.57 | 5.41 | 5.16 |
| | $R_{wF}$ | 3.91 | 3.87 | 3.8 |
| | $R_{wF}(I_{obs}>3\sigma_{obs})$ | 3.79 | 3.61 | 3.39 |
| | Extinction | 0.047(3) | 0.079(6) | 0.130(6) |
| Neutron | $R_F$ | 8.4 | 10.5 | 12.28 |
| | $R_F(I_{obs}>3\sigma_{obs})$ | 5.57 | 5.41 | 5.16 |
| | $R_{wF}$ | 3.91 | 3.87 | 3.8 |
| | $R_{wF}(I_{obs}>3\sigma_{obs})$ | 3.79 | 3.61 | 3.39 |
| | Extinction | 0.040(6) | 0.053(3) | 0.052(3) |
| Ba 8c | x | 0.81534(2) | 0.81518(2) | 0.81509(3) |
| | $U_{11}$ | 0.0270(1) | 0.0360(1) | 0.0453(1) |
| | $U_{12}$ | -0.00746(8) | -0.00945(9) | -0.0114(1) |
| Sn/Ga(1) 12d | ai[Sn1] | 0.207(1) | 0.208(1) | 0.206(1) |
| | $U_{11}$ | 0.0112(1) | 0.0144(1) | 0.0178(1) |
| | $U_{22}$ | 0.0168(1) | 0.0211(1) | 0.0257(1) |
| Sn/Ga(2) 2a | ai[Sn2] | 0.0320(5) | 0.0322(5) | 0.0329(5) |
| | $U_{11}$ | 0.0083(1) | 0.0113(2) | 0.0146(2) |
| Sn/Ga(3) 24g | ai[Ga3] | 0.158(2) | 0.160(2) | 0.163(2) |
| | ai[Sn3] | 0.340(1) | 0.338(1) | 0.336(1) |
| | x | 0.58436(2) | 0.58433(2) | 0.58430(2) |
| | z | 0.85135(2) | 0.85140(2) | 0.85141(2) |
| | $U_{11}$ | 0.01130(6) | 0.01538(7) | 0.01981(8) |
| | $U_{33}$ | 0.00979(9) | 0.01262(9) | 0.01608(10) |
| | $U_{12}$ | -0.00014(6) | -0.00042(7) | -0.00052(8) |
| | $U_{13}$ | 0.00003(4) | -0.00001(4) | 0.00006(5) |
| Sn/Ga(3) 8c | X | 0.63423(2) | 0.63420(2) | 0.63423(2) |
| | $U_{11}$ | 0.0090(1) | 0.0121(1) | 0.0160(1) |
| | $U_{12}$ | 0.00004(7) | 0.00000(7) | -0.00003(8) |

**Symmetry constraints**

**Positions:**

1BGS – "*Anharmonic*" and "*Anisotropic*" models:

| | |
|---|---|
| Ba(1) 2a: | x=y=z=0 |
| Ba(2) 6d: | x=1/4, y=1/2, z=0 |
| Sn/Ga(1) 6c: | x=1/4, y=0, z=1/2 |
| Sn/Ga(2) 16i: | x=y=z |
| Sn/Ga(3) 24k: | x=0 |

1BGS – "*24k*" model:

| | |
|---|---|
| Ba(1) 2a: | x=y=z=0 |
| Ba(2) 24k: | z=0 |
| Sn/Ga(1) 6c: | x=1/4, y=0, z=1/2 |
| Sn/Ga(2) 16i: | x=y=z |
| Sn/Ga(3) 24k: | x=0 |

8BGS:

| | |
|---|---|
| Ba 8c: | x=y=z |
| Sn/Ga(1) 12d: | x=3/4, y=1/2, z=0 |
| Sn/Ga(2) 2a: | x=y=z=0 |
| Sn/Ga(3) 24g: | x=y |
| Sn/Ga(4) 8c: | x=y=z |

**Occupancies – separate refinements:**

1BGS:

| | |
|---|---|
| Sn/Ga(1) 6c: | ai[Sn1]=0.125-ai[Ga1] |
| Sn/Ga(2) 16i: | ai[Sn2]=0.333-ai[Ga2] |
| Sn/Ga(3) 24k: | (ai[Sn3]=0.5-ai[Ga3])* |
| | ai[Sn3]=30/48-ai[Sn1]-ai[Sn2] |
| | ai[Ga3]=16/48-ai[Ga1]-ai[Ga2] |

8BGS:

| | |
|---|---|
| Sn/Ga(1) 12d: | ai[Ga1]=0.25-ai[Sn1] |
| Sn/Ga(2) 2a: | ai[Ga2]=0.041667-ai[Sn2] |
| Sn/Ga(3)24g: | (ai[Ga3]=0.5-ai[Sn3])* |
| Sn/Ga(4) 8c: | ai[Ga4]=0.16666667-ai[Sn4] |
| | ai[Sn3]=30/48-ai[Sn1]-ai[Sn2]-ai[Sn4] |
| | ai[Ga3]=16/48-ai[Ga1]-ai[Ga2]-ai[Ga4] |

*Redundant constraints

**Occupancies – Joint neutron and x-ray refinements**

1BGS:

| | |
|---|---|
| Sn/Ga(1) 6c: | - |
| Sn/Ga(2) 16i: | ai[Sn2]=0.333-ai[Ga2] |

| | |
|---|---|
| Sn/Ga(3) 24k: | ai[Sn3]=0.5-ai[Ga3] |
| | ai[Sn3]=30/48-ai[Sn1]-ai[Sn2] |

8BGS:

| | |
|---|---|
| Sn/Ga(1) 12d: | ai[Ga1]=0.25-ai[Sn1] |
| Sn/Ga(2) 2a: | ai[Ga2]=0.041667-ai[Sn2] |
| Sn/Ga(3)24g: | - |
| Sn/Ga(4) 8c: | ai[Ga4]=0.16666667-ai[Sn4] |
| | ai[Sn4]=30/48-ai[Sn1]-ai[Sn2]-ai[Sn3] |

**Anharmonic ADPs for guest atoms**

1BGS:

$U_{22}=U_{33}$, $U_{12}=U_{13}=U_{23}=0$,

$C_{111}=C_{112}=C_{113}=C_{123}=0$, $C_{122}=-C_{133}$, $C_{222}=C_{223}=C_{233}=C_{333}=0$

$D_{1112}=D_{1113}=D_{1123}=0$, $D_{1122}=D_{1133}$, $D_{1222}=D_{1223}=D_{1233}=D_{1333}=D_{2223}=D_{2333}=0$, $D_{3333}=D_{2222}$

8BGS:

$U_{33}=U_{22}= U_{11}$, $U_{23}= U_{13}=U_{12}$

$C_{113}= C_{122}= C_{133}= C_{223}= C_{233}=C_{112}$, $C_{222}= C_{333}=C_{111}$

$D_{1113}= D_{1222}= D_{1333}= D_{2223}= D_{2333}=D_{1112}$, $D_{1133}= D_{2233}=D_{1122}$, $D_{1223}= D_{1233}=D_{1123}$, $D_{3333}=D_{2222}=D_{1111}$