Supplementary Materials

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Synopsis

Synchrotron PXRD data are analyzed with generally available Rietveld refinement software and strategies are suggested for subsequent calculation of maximum entropy method charge densities.

Abstract

Structure factor extractions in commonly used Rietveld refinement programs (FullProf, Jana2006 and GSAS) were examined with respect to subsequent calculation of electron density distributions (EDD) using the maximum entropy method (MEM). As a test case 90 K synchrotron powder X-ray diffraction (PXRD) data were collected on the potential hydrogen storage material, $NaGaH_4$, at SPring8, Japan. To support the model, neutron powder diffraction data were collected on the fully deuterated sample at PSI, Switzerland. Firstly, it was established whether the programs can produce observed structure factors, F_{obs}, corrected for anomalous dispersion and scaled to the scattering power of one unit cell. Secondly, different models for background and peak shape description were investigated with respect to the extracted F_{obs}, and the effect on the subsequent MEM EDDs were analysed within the quantum theory of atoms in molecules. Substantial differences are observed in the estimated standard deviations, σ_{obs}, produced by the different programs. Since σ_{obs} is a vital parameter in the calculation of MEM EDDs this leads to substantial variation between the MEM EDDs obtained with different Rietveld programs even in cases with similar F_{obs}. A new approach for selecting an optimised MEM EDD and thereby minimising the effect of variation in σ_{obs} is suggested.

1. Rietveld refinements

This section contains diffractograms of all the refinements discussed in the article, see Figure 1-11. The nomenclature of the refinements is preserved and detailed information about the refinements and their differences are found in the main article. In the FullProf diffractograms, the collected intensity is indicated by a red colour, the calculated intensity by a black colour and the difference between these two by a blue colour. GSAS employs a similar colour scheme, but its diffractograms contains additional information as the modelled background is demonstrated by a green line. The diffractograms of Jana2006 are in black and white. The collected intensity is the dotted line, the calculated intensity is the solid line and the difference between these two is the solid line beneath the diffractograms. As **F2** and **FP2** are identical, only the diffractogram of **F2** is provided.

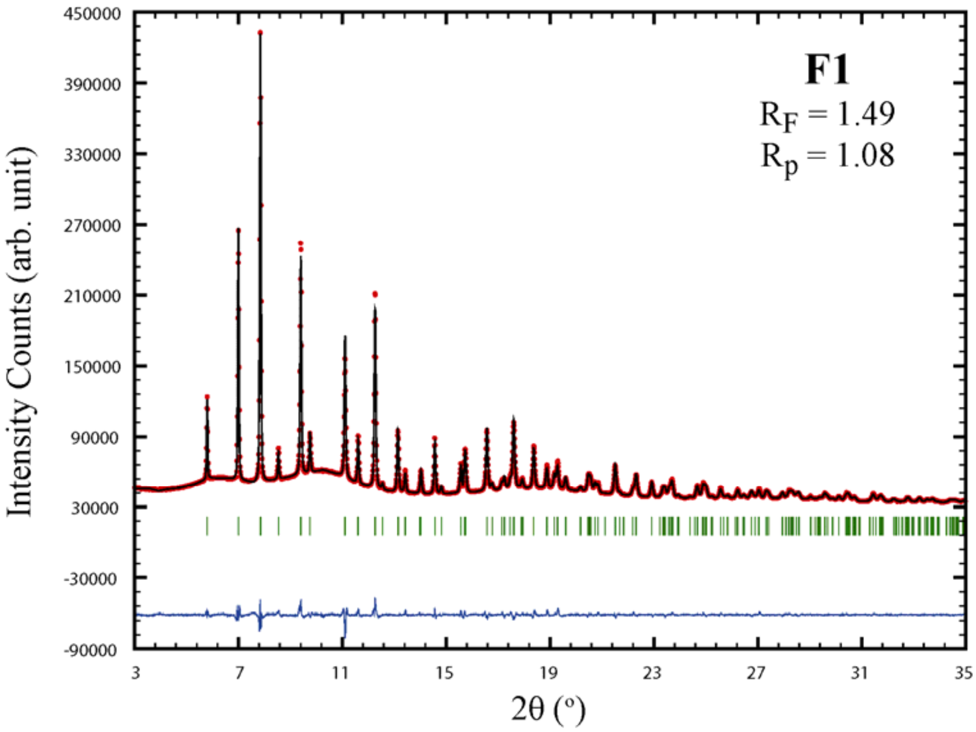

Figure 1

The FullProf refinement, **F1**, in which the background is approximated by linear interpolation consisting of 56 automatically selected points. Their intensity height has been adjusted.

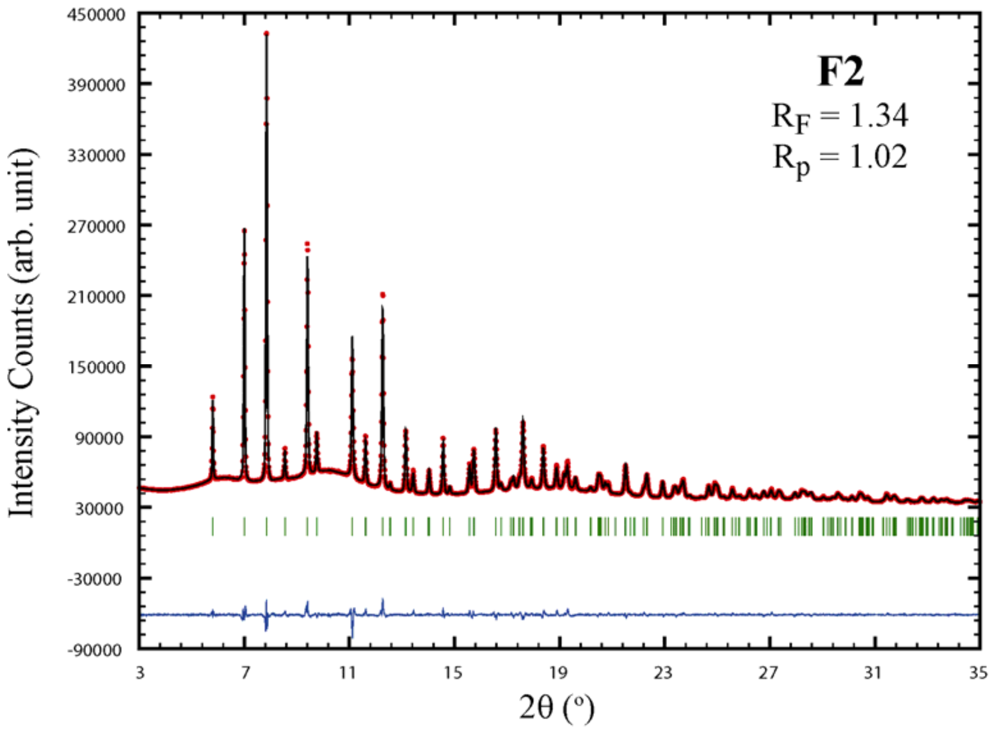

Figure 2

The FullProf refinement, **F2**, in which the background is approximated by linear interpolation consisting of 84 manually selected points. Their intensity height has been adjusted. **F2** and **FP2** are identical.

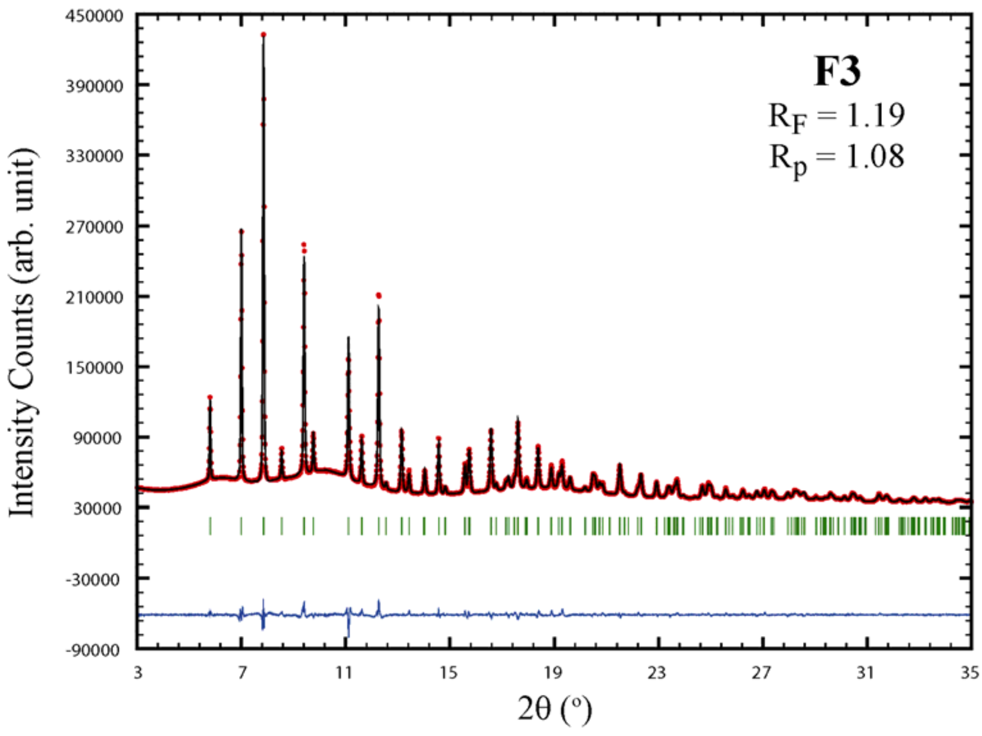

Figure 3

The FullProf refinement, **F3**, in which the employment of iterative Fourier filtering renders the background approximation smoother. The background of **F2** is utilised as starting point for the iteration.

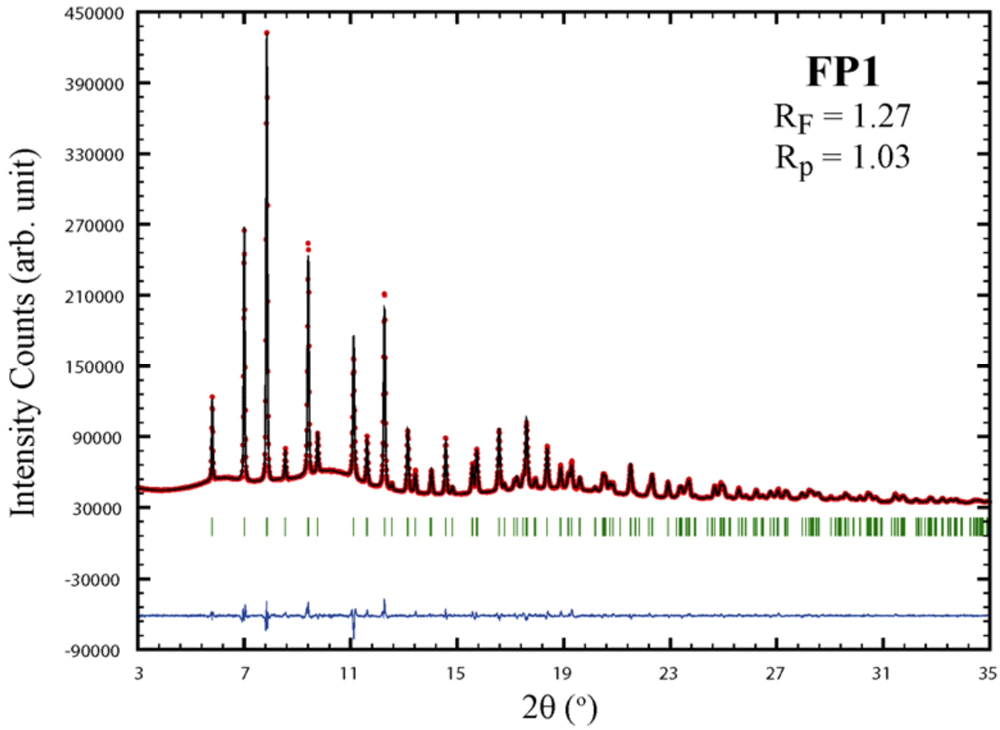

Figure 4

The FullProf refinement, **FP1**. The peak shape is modelled with a pseudo-Voigt function and the background by linear interpolation consisting of 84 manually selected points.

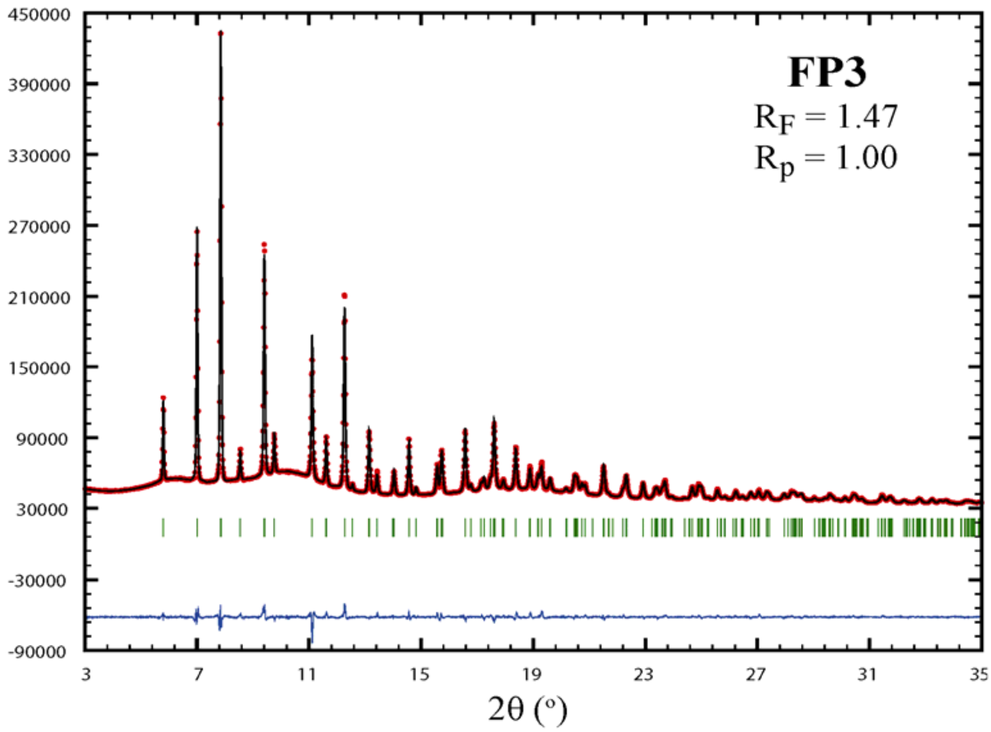

Figure 5

The FullProf refinement, **FP3**. The peak shape is modelled with a Pearson VII function and the background by linear interpolation consisting of 84 manually selected points.

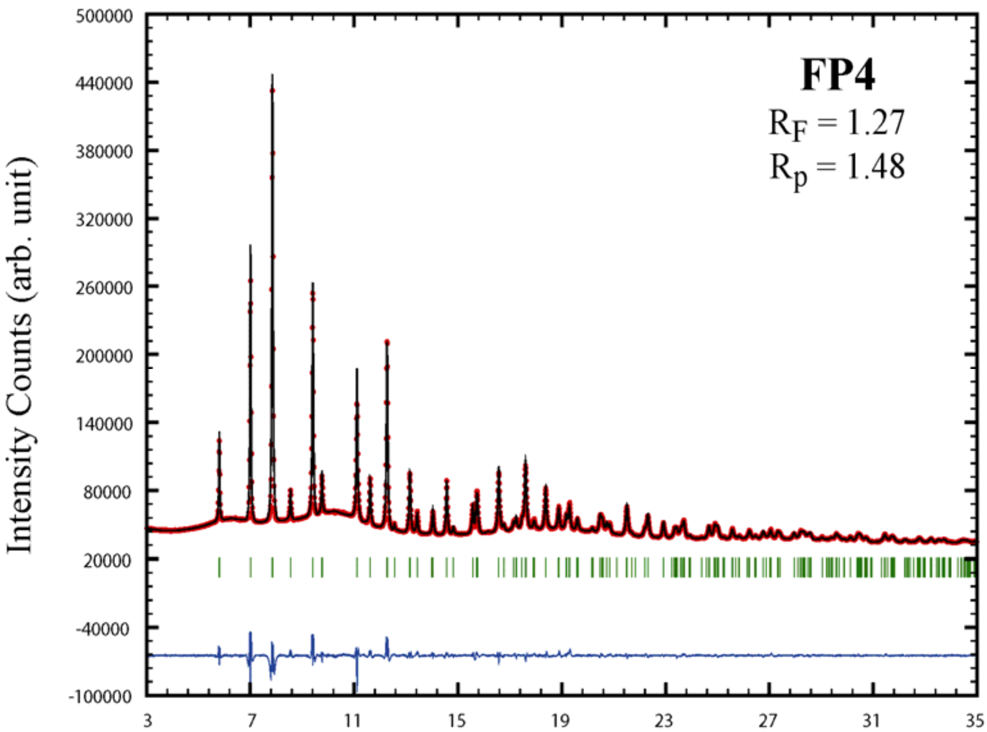

Figure 6

The FullProf refinement, **FP4**. The peak shape is modelled with a Lorentzian function and the background by linear interpolation consisting of 84 manually selected points.

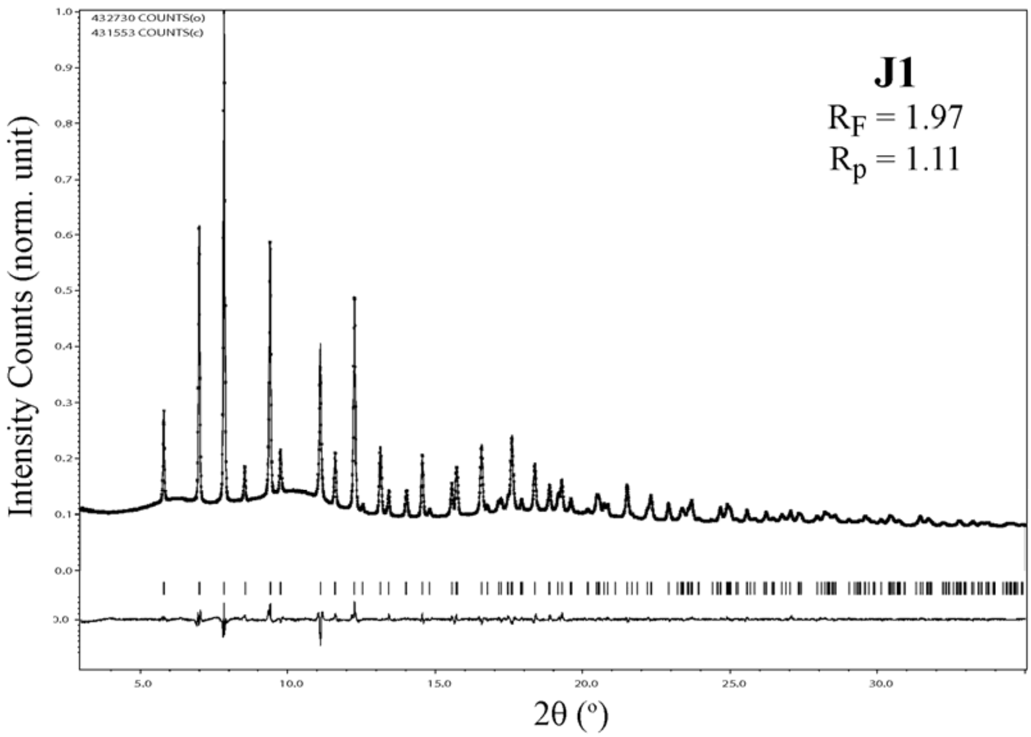

Figure 7

The Jana2006 refinement, **J1**, in which the background is approximated by linear interpolation consisting of 56 automatically selected points. The modelled background is identical to that of **F1**.

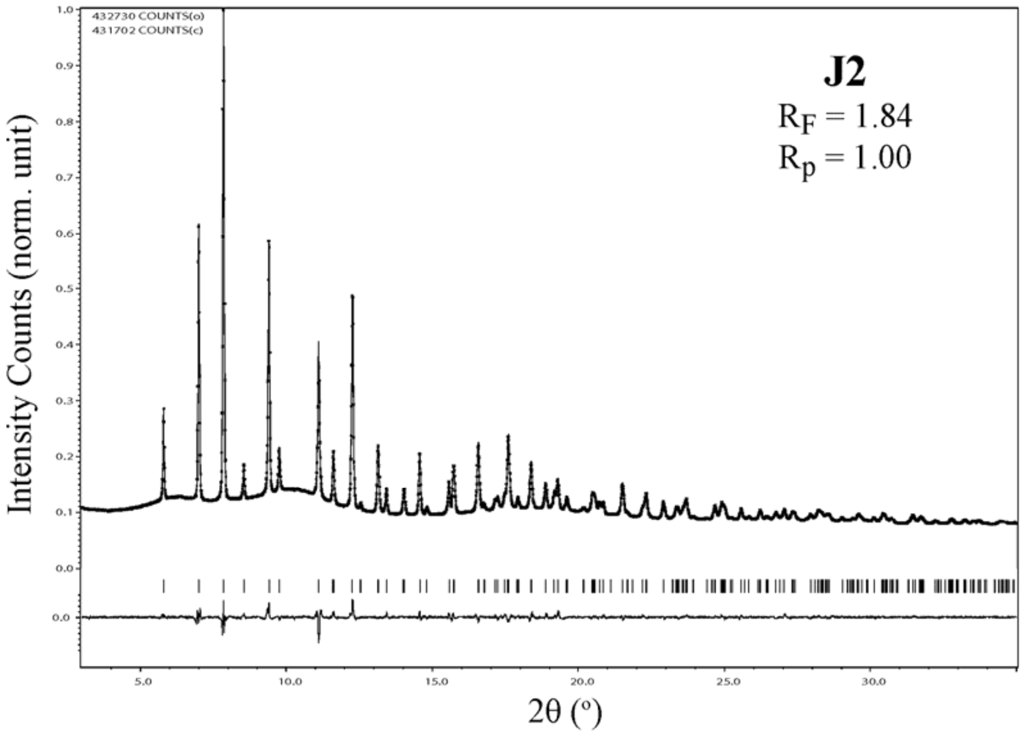

Figure 8

The Jana2006 refinement, **J2**, in which the background is approximated by linear interpolation consisting of 84 manually selected points. The modelled background is identical to that of **F2**.

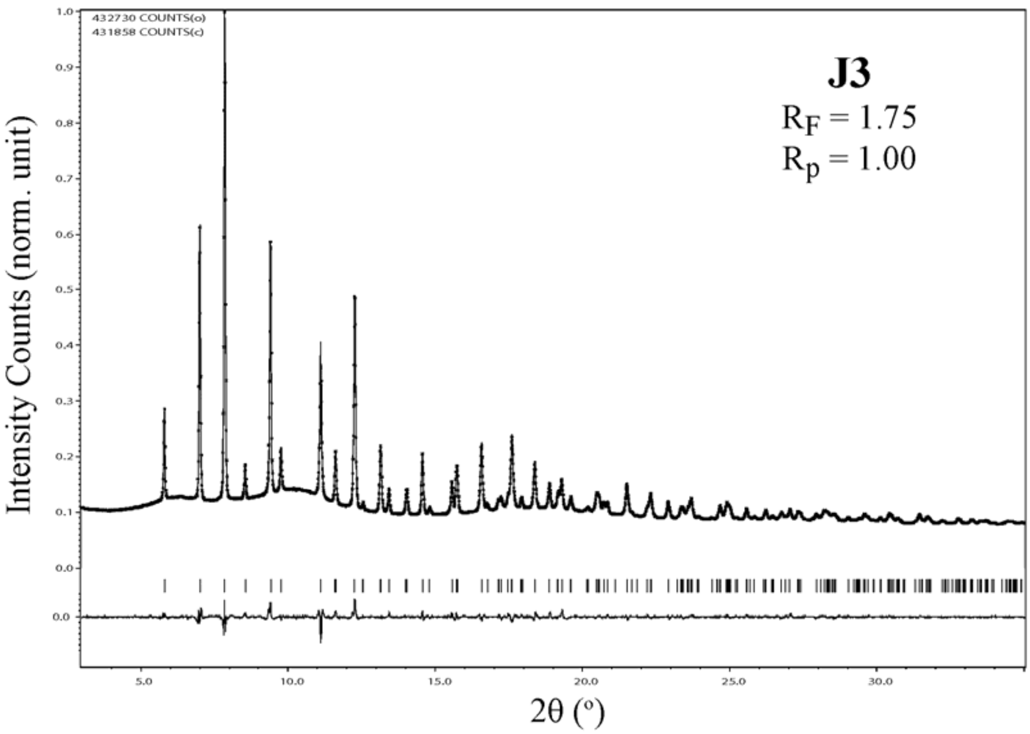

Figure 9

The Jana2006 refinement, **J3**, in which the background approximation is fabricated by combining the linear interpolation model used in **J2** with a Legendre polynomial consisting of 23 adjustable coefficients.

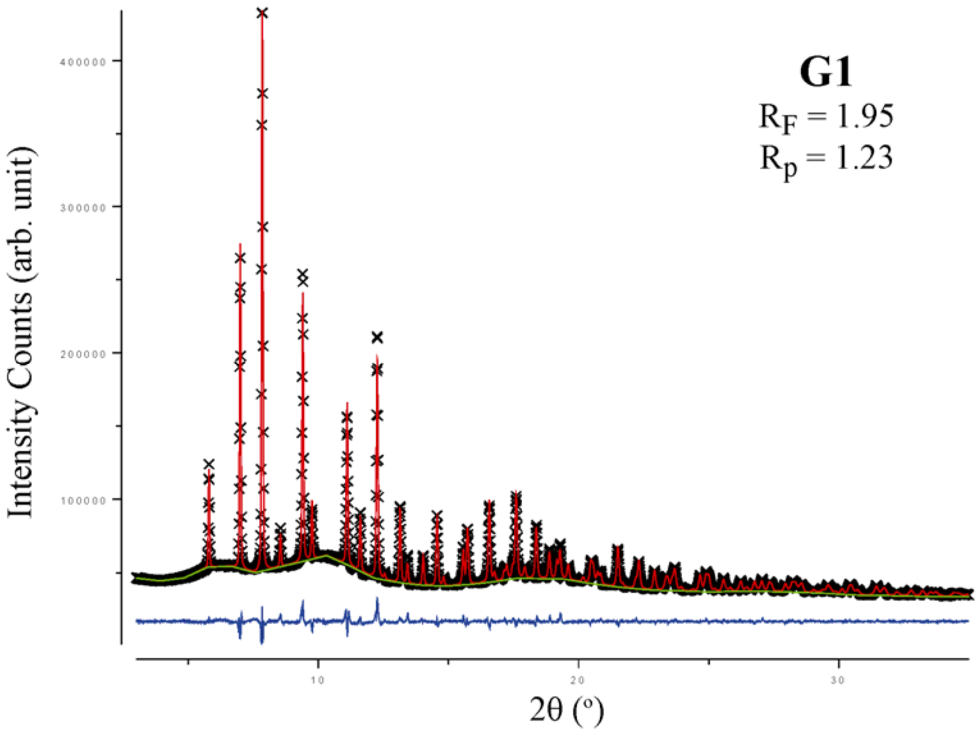

Figure 10

The GSAS+EXPGUI refinement, **G1**, in which the background approximation is fabricated by linear interpolation utilising the maximum number of 36 terms.

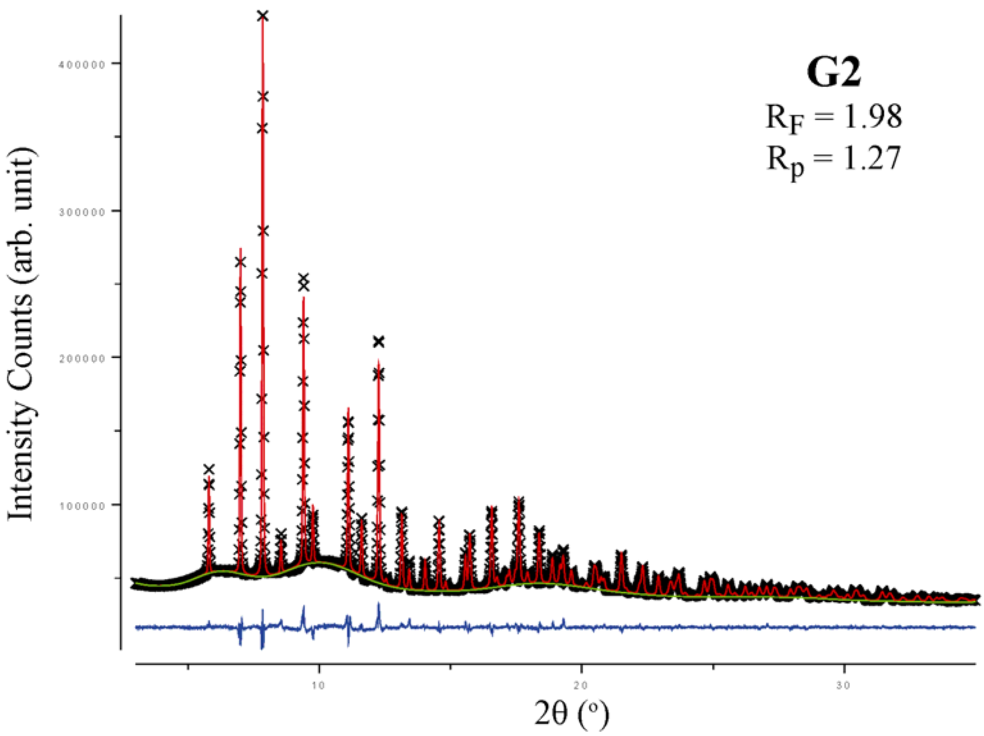

Figure 11

The GSAS+EXPGUI refinement, **G2**, in which the background approximation is fabricated by a Chebyshev polynomial consisting of 27 adjustable coefficients.

2. Calculation of anomalous dispersion reference

If $\boldsymbol{H}$ is the scattering vector, $\boldsymbol{x}$ is the atomic position vector and isotropic vibration is described by the temperature factor B_{iso}, a general expressions for the structure factor is given by

$$F_{\boldsymbol{H}} = \sum_{j=1}^{N} f_j exp(2\pi i\boldsymbol{H} \cdot \boldsymbol{x_j}) \exp\left(-B_{iso,j}\frac{sin^2\theta}{\lambda^2}\right) = A_{\boldsymbol{H}} + iB_{\boldsymbol{H}}$$

where the real and imaginary part are expressed by

$$A_{\boldsymbol{H}} = \sum_{j=1}^{N} f_j cos(2\pi i\boldsymbol{H} \cdot \boldsymbol{x_j})\exp\left(-B_{iso,j}\frac{sin^2\theta}{\lambda^2}\right)$$

$$B_{\boldsymbol{H}} = \sum_{j=1}^{N} f_j sin(2\pi i\boldsymbol{H} \cdot \boldsymbol{x_j})\exp\left(-B_{iso,j}\frac{sin^2\theta}{\lambda^2}\right)$$

The summation runs through all N atoms of the unit cell. When anomalous dispersion is taken into account, the atomic scattering factor, f, becomes complex and is written as

$$f = f_0 + f_1 + if_2 = f' + if''$$

where f_0 is the normal atomic scattering factor. f_1 and f_2 are, respectively, the real and imaginary modifications in the atomic scattering factor due to anomalous dispersion (AD). In order to simplify, the real parts are grouped into f', and the imaginary part is relabelled to f''. Insertion of this expression into the general structure factor expression provides an evident separation of the real and imaginary parts:

$$F_{\boldsymbol{H}} = \sum_{j=1}^{N} f_j' exp(2\pi i\boldsymbol{H} \cdot \boldsymbol{x_j}) \exp\left(-B_{iso,j}\frac{sin^2\theta}{\lambda^2}\right) + i\sum_{j=1}^{N} f_j'' exp(2\pi i\boldsymbol{H} \cdot \boldsymbol{x_j})\exp\left(-B_{iso,j}\frac{sin^2\theta}{\lambda^2}\right)$$

The AD superscript denotes the terms that contain anomalous scattering contributions. As the structure of $NaGaH_4$ is centrosymmetric, the structure factor is in our case reduced to

$$F_{\boldsymbol{H}} = A_1 + iA_2$$

The observed structure factors extracted from our experimental PXRD data corresponds to the above expression. Utilising the refinement model, it is possible to remove their AD contributions utilising the following correction scheme:

$$A_{obs}^0 = \frac{A_{calc}^{AD}}{F_{calc}^{AD}} F_{obs}^{AD} - A_{calc}^{AD} - A_{calc}^0 = A_{obs}^{AD} - A_{calc}^{AD} - A_{calc}^0$$

$$B_{obs}^0 = \frac{B_{calc}^{AD}}{F_{calc}^{AD}} F_{obs}^{AD} - B_{calc}^{AD} - B_{calc}^0 = B_{obs}^{AD} - B_{calc}^{AD} - B_{calc}^0$$

where the 0 superscript is used to designate terms without anomalous dispersion. In section 4.1 of the main article, it is investigated whether or not the three refinement programs correctly remove AD on the basis of the structure factor difference:

$$\Delta F_{obs}(\boldsymbol{H}) = |F_{obs}(\boldsymbol{H})|_{mAD} - |F_{obs}(\boldsymbol{H})|_{m0}$$

where $|F_{obs}(\boldsymbol{H})|_{mAD}$ are the magnitude of the extracted, observed structure factors obtained from a refinement model that describes AD. In the case of $|F_{obs}(\boldsymbol{H})|_{m0}$ the AD parameters of the refinement model are set equal to zero. Compared to eq. (6) in the article the labelling scheme has been extended in order to precisely define the structure factors. To summarize, the superscripts, 0 and AD, are used to denoted whether or not structure factors contain AD, whereas the subscripts, $m0$ and mAD, are applied to observed structure factors in order to clarify whether or not their extraction model describes AD. The latter influences the decomposition of overlapping reflections as well as the phases assigned to the observed reflections. If the refinement software performs the AD correction correctly, the structure factor difference becomes:

$$\begin{aligned}\Delta F_{obs}(\boldsymbol{H}) &= \left|F^{0}_{obs}(\boldsymbol{H})\right|_{mAD} - \left|F^{AD}_{obs}(\boldsymbol{H})\right|_{m0} \\ &= \sqrt{[(A^{AD}_{obs})_{mAD} - A^{AD}_{calc} - A^{0}_{calc}]^2 + [(B^{AD}_{obs})_{mAD} - B^{AD}_{calc} - B^{0}_{calc}]^2} - \left|A^{AD}_{obs}\right|_{m0} \\ &= \sqrt{[(A^{AD}_{obs})_{mAD} - A_1 - A_0]^2 + [(B^{AD}_{obs})_{mAD} - A_2]^2} - \left|A^{AD}_{obs}\right|_{m0}\end{aligned}$$

It can be seen from the latter expression that $\Delta F_{obs}(\boldsymbol{H})$ is dominated by the term, $A_1 - A_0$. Moreover, the latter demonstrates how the reference, $\Delta F_{ref}(\boldsymbol{H})$, is calculated. The correction terms are simply computed from the AD parameters:

$$A_1 - A_0 = \sum_{j=1}^{N} f_{1,j} cos\left(2\pi i\boldsymbol{H}\cdot\boldsymbol{x_j}\right) \exp\left(-B_{iso,j}\frac{sin^2\theta}{\lambda^2}\right)$$

$$A_2 = \sum_{j=1}^{N} f_{2,j} cos\left(2\pi i\boldsymbol{H}\cdot\boldsymbol{x_j}\right) \exp\left(-B_{iso,j}\frac{sin^2\theta}{\lambda^2}\right)$$

whereas the remaining terms are based on a set of $F^{AD}_{obs}(\boldsymbol{H})$ extracted from the PXRD data. Utilising external software, XD2006 (Volkov *et al.*, 2006), $F^{AD}_{obs}(\boldsymbol{H})$ is divided into its real and imaginary parts in accordance with the given model. E.g. for a centrosymmetric structure the imaginary terms of the structure factor adds up to zero when the model does not describe AD, i.e. $\left|F^{AD}_{obs}(\boldsymbol{H})\right|_{m0} = \left|A^{AD}_{obs}(\boldsymbol{H})\right|_{m0}$. The shortcoming of this approach is that differences originating from the decomposition of overlapping reflections are not taken into account. However, if the refinement software correctly removes AD a close match is still anticipated for single peaks in the low-order region. The remaining reflections ought to agree qualitatively with the reference.

XD2006: Volkov, A., Macchi, P., Farrugia, L. J., Gatti, C., Mallinson, P., Richter, T. & Koritsanszky, T. (2006)

3. Optimal electron densities

A detailed view on the optimisation procedure for the refinements, **F1-3**, **J1-3** and **G1-2**, is provided in Figure 12-14. These figures illustrate how Gaussian the residual EDD (invers Fourier transformation of $F_{obs} - F_{MEM}$) is at different MEM stopping points. The optimized χ^2_{aim} corresponds to the most Gaussian residual EDD, i.e. it is defined by the point, where the coefficients of determination curve has its maximum. If several maxima of equal magnitude are observed, the maximum at the lowest χ^2_{aim}-value is chosen.

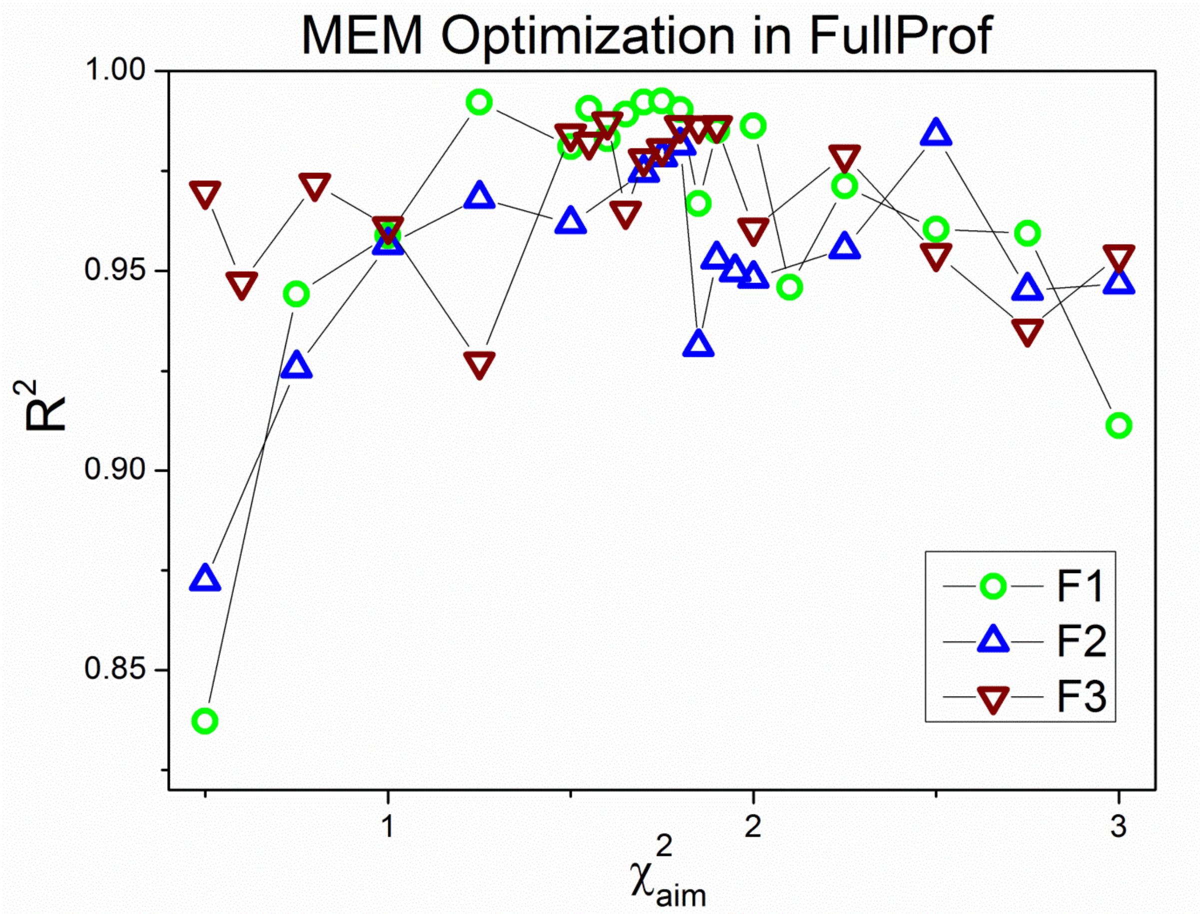

Figure 12

Coefficients of determination, R^2, obtained by fitting fractal dimension distributions to a parabolic function, $f(x) = c \cdot x^2$.

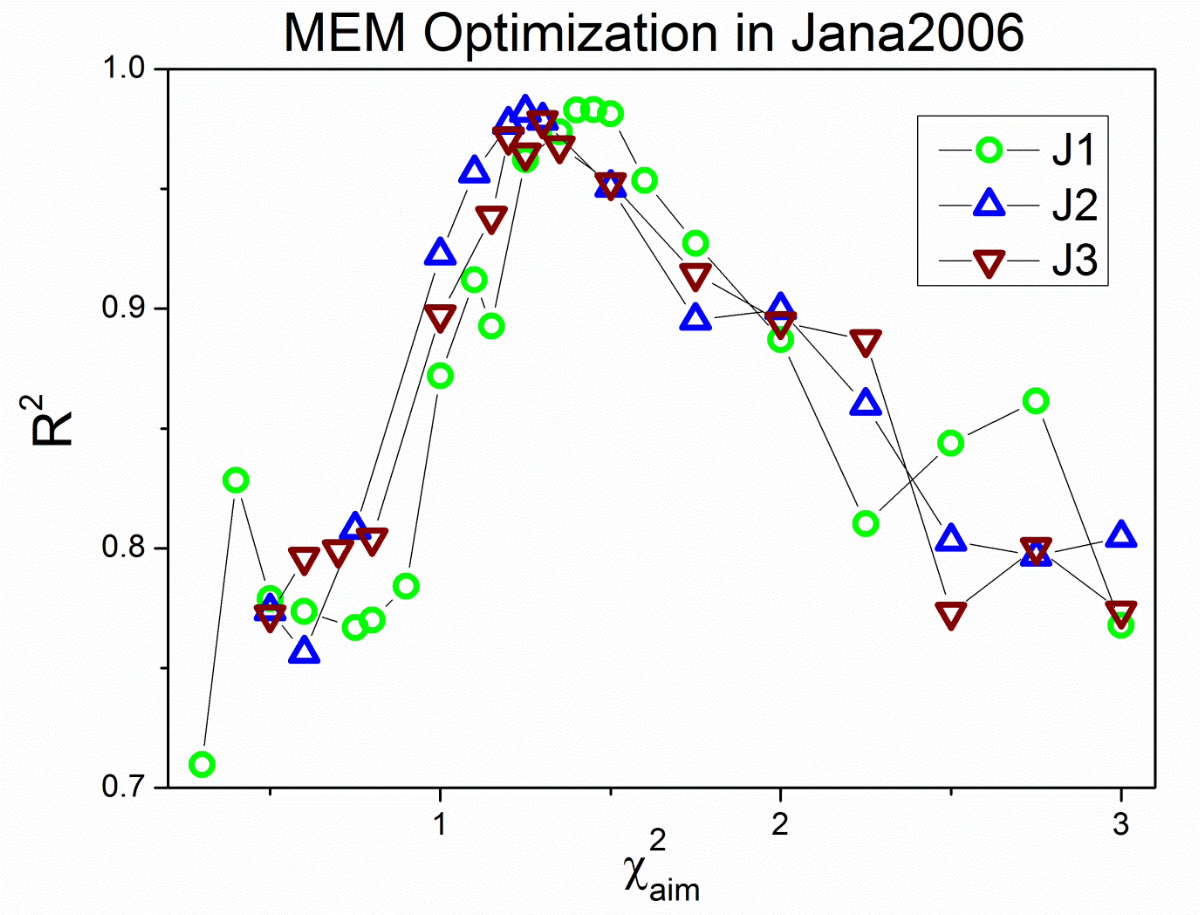

Figure 13

Coefficients of determination, R^2, obtained by fitting fractal dimension distributions to a parabolic function, $f(x) = c \cdot x^2$.

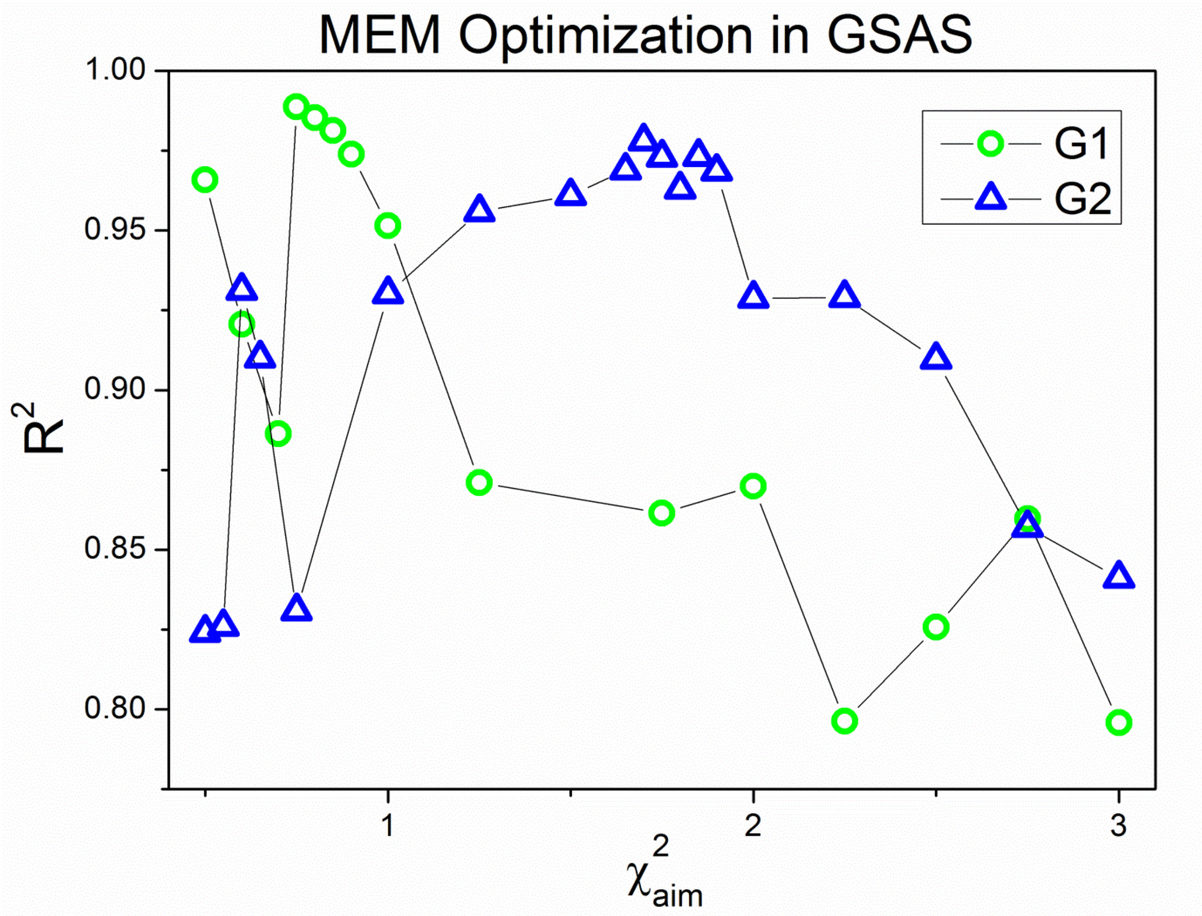

Figure 14

Coefficients of determination, R^2, obtained by fitting fractal dimension distributions to a parabolic function, $f(x) = c \cdot x^2$.

4. Structure factor outputs

The 80 first $F_{obs}(\boldsymbol{H})$ and their standard uncertainties, $\sigma_{obs}(\boldsymbol{H})$, are listed in the following tables for the refinements, **F1-3**, **FP1-4**, **J1-3** and **G1-2**. As the $NaGaH_4$ crystal structure is centrosymmetric, the phases are simply given by the sign of $F_{obs}(\boldsymbol{H})$. The extracted $F_{obs}(\boldsymbol{H})$ of GSAS and FullProf have been subjected to post treatment in XD2006 in order to correct for anomalous dispersion. In addition this also brought the $F_{obs}(\boldsymbol{H})$ of GSAS on absolute scale. Thus, the listed $F_{obs}(\boldsymbol{H})$ correspond to those used for MEM reconstruction of the electron density distributions.

FullProf refinement **F1**									
h	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	*h*	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	40.4905	0.2130	4	2	2	37.0002	0.2443
1	1	1	64.4224	0.0874	3	1	4	26.7336	0.3319
0	0	2	-143.9630	0.0933	5	1	0	28.6073	0.3435
2	0	0	143.8140	0.0933	2	4	2	62.8383	0.2187
0	2	0	-58.3250	0.2346	1	1	5	44.8797	0.1222
0	2	1	125.9630	0.1334	5	1	1	44.3712	0.1481
1	1	2	-39.3199	0.1354	1	3	4	-50.5563	0.2227
2	0	2	-121.5260	0.1936	0	4	3	70.5692	0.3772
0	2	2	46.7028	0.1208	3	3	3	-6.5041	0.3009
2	2	0	-57.9451	0.1503	0	2	5	80.5422	0.2327
2	2	1	115.2270	0.1043	4	2	3	-81.3641	0.2176
3	1	0	28.2274	0.2828	5	1	2	-28.5699	0.2893
1	1	3	-49.5671	0.0996	1	5	0	15.1583	0.4297
3	1	1	53.4811	0.1036	1	5	1	-47.9260	0.2536
1	3	0	-59.2645	0.2446	2	4	3	64.6378	0.1905
1	3	1	7.3092	0.0511	4	0	4	85.1557	0.2759
2	2	2	49.0303	0.1960	2	2	5	76.2966	0.3283
0	2	3	-107.7920	0.2337	1	5	2	-15.9995	0.2177
3	1	2	-29.9753	0.2396	0	4	4	-54.8319	0.2535
1	3	2	59.5913	0.1741	4	4	0	-55.2332	0.2195
0	0	4	112.6220	0.2337	3	1	5	39.7141	0.1497
4	0	0	112.4910	0.2653	5	1	3	-38.2955	0.1572
2	2	3	-99.4189	0.1770	3	3	4	-47.9908	0.1702
1	1	4	30.7746	0.2387	5	3	0	-45.7934	0.1449
0	4	0	-71.3783	0.4108	0	0	6	-84.6775	0.2140
3	1	3	-44.8947	0.2007	4	4	1	-61.3199	0.1649
3	3	0	-57.7609	0.2169	6	0	0	84.5638	0.2852
0	4	1	-74.6544	0.0984	1	3	5	5.4724	0.0767
2	0	4	101.1050	0.1313	5	3	1	5.6903	0.0794
4	0	2	-101.3290	0.1462	4	2	4	-31.4268	0.4513
1	3	3	-7.7503	0.0625	1	1	6	-24.7155	0.5034
3	3	1	6.0136	0.0405	3	5	0	12.4313	0.1789
0	2	4	-40.0153	0.2368	2	4	4	-52.9510	0.2252
4	2	0	-43.8368	0.2726	4	4	2	52.7713	0.2117
4	2	1	91.5901	0.2217	1	5	3	43.4760	0.1375
0	4	2	66.1781	0.2398	3	5	1	-44.0660	0.1306
2	4	0	-68.4936	0.2441	5	3	2	45.3430	0.1222
3	3	2	55.2671	0.2083	2	0	6	-76.6099	0.2283
2	4	1	-74.7050	0.1911	6	0	2	-75.9201	0.3033
2	2	4	-37.9059	0.2453	0	2	6	31.5539	0.3898

FullProf refinement **F2** / **FP2**									
h	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	*h*	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	40.6384	0.2112	4	2	2	37.3694	0.2379
1	1	1	64.4085	0.0872	3	1	4	26.5015	0.3362
0	0	2	-143.2080	0.0942	5	1	0	28.5128	0.3440
2	0	0	143.1960	0.0940	2	4	2	63.1484	0.2172
0	2	0	-56.5927	0.2479	1	1	5	44.8387	0.1216
0	2	1	126.1400	0.1329	5	1	1	44.3228	0.1474
1	1	2	-39.0059	0.1374	1	3	4	-50.3750	0.2233
2	0	2	-121.7050	0.1927	0	4	3	69.9079	0.3823
0	2	2	46.6600	0.1202	3	3	3	-6.4344	0.3103
2	2	0	-58.0639	0.1489	0	2	5	80.8723	0.2306
2	2	1	115.1340	0.1045	4	2	3	-81.6240	0.2161
3	1	0	28.6428	0.2732	5	1	2	-28.4610	0.2893
1	1	3	-49.5282	0.0995	1	5	0	14.9100	0.4321
3	1	1	53.3895	0.1036	1	5	1	-47.8930	0.2528
1	3	0	-59.3855	0.2428	2	4	3	64.5881	0.1897
1	3	1	7.2690	0.0528	4	0	4	85.3099	0.2750
2	2	2	48.3295	0.2006	2	2	5	76.2759	0.3283
0	2	3	-108.5780	0.2299	1	5	2	-15.9234	0.2136
3	1	2	-29.9148	0.2396	0	4	4	-55.0060	0.2531
1	3	2	59.5780	0.1734	4	4	0	-55.4074	0.2192
0	0	4	112.9990	0.2317	3	1	5	39.6607	0.1490
4	0	0	113.0490	0.2619	5	1	3	-38.2492	0.1564
2	2	3	-99.4757	0.1767	3	3	4	-47.9487	0.1695
1	1	4	31.2532	0.2300	5	3	0	-45.7498	0.1443
0	4	0	-70.6537	0.4203	0	0	6	-84.7518	0.2139
3	1	3	-44.5190	0.2030	4	4	1	-61.2159	0.1645
3	3	0	-57.5647	0.2169	6	0	0	84.6099	0.2847
0	4	1	-74.5266	0.0979	1	3	5	5.5078	0.0772
2	0	4	101.1990	0.1310	5	3	1	5.7240	0.0800
4	0	2	-101.4500	0.1457	4	2	4	-31.2989	0.4507
1	3	3	-7.8529	0.0619	1	1	6	-24.9537	0.4898
3	3	1	6.0890	0.0405	3	5	0	12.4829	0.1711
0	2	4	-39.9309	0.2356	2	4	4	-53.2434	0.2234
4	2	0	-43.5131	0.2745	4	4	2	53.0377	0.2102
4	2	1	91.9018	0.2200	1	5	3	43.4901	0.1366
0	4	2	66.2108	0.2402	3	5	1	-44.0758	0.1300
2	4	0	-68.5052	0.2446	5	3	2	45.3042	0.1216
3	3	2	55.0861	0.2088	2	0	6	-76.6386	0.2280
2	4	1	-74.3975	0.1918	6	0	2	-75.9042	0.3029
2	2	4	-38.1677	0.2405	0	2	6	31.3147	0.3915

FullProf refinement **F3**									
h	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	*h*	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	40.5648	0.2104	4	2	2	37.3185	0.2375
1	1	1	64.2430	0.0871	3	1	4	26.6398	0.3277
0	0	2	-144.7870	0.0912	5	1	0	28.6275	0.3363
2	0	0	144.7760	0.0911	2	4	2	62.9337	0.2155
0	2	0	-56.4656	0.2486	1	1	5	44.7692	0.1212
0	2	1	124.6530	0.1353	5	1	1	44.2042	0.1468
1	1	2	-38.4984	0.1399	1	3	4	-50.0950	0.2229
2	0	2	-123.8160	0.1846	0	4	3	69.6119	0.3833
0	2	2	46.7955	0.1193	3	3	3	-6.2820	0.3057
2	2	0	-58.0679	0.1484	0	2	5	80.8894	0.2287
2	2	1	113.1140	0.1077	4	2	3	-81.6588	0.2144
3	1	0	26.5667	0.3127	5	1	2	-28.5209	0.2818
1	1	3	-49.6081	0.0984	1	5	0	15.1803	0.4124
3	1	1	53.4858	0.1024	1	5	1	-47.7964	0.2493
1	3	0	-59.5694	0.2390	2	4	3	64.6677	0.1892
1	3	1	7.0407	0.0532	4	0	4	85.1488	0.2731
2	2	2	47.7719	0.2052	2	2	5	76.2122	0.3256
0	2	3	-108.3870	0.2290	1	5	2	-15.9868	0.2107
3	1	2	-29.9424	0.2361	0	4	4	-54.8074	0.2503
1	3	2	59.1252	0.1745	4	4	0	-55.2083	0.2170
0	0	4	112.6490	0.2315	3	1	5	39.6054	0.1479
4	0	0	112.7420	0.2615	5	1	3	-38.1754	0.1554
2	2	3	-99.6261	0.1748	3	3	4	-47.7481	0.1687
1	1	4	31.3028	0.2252	5	3	0	-45.5516	0.1437
0	4	0	-70.7987	0.4106	0	0	6	-84.3811	0.2138
3	1	3	-44.7460	0.1988	4	4	1	-61.1004	0.1649
3	3	0	-57.7444	0.2115	6	0	0	84.1382	0.2845
0	4	1	-74.9424	0.0969	1	3	5	5.3496	0.0770
2	0	4	101.4600	0.1294	5	3	1	5.5595	0.0800
4	0	2	-101.7500	0.1436	4	2	4	-30.8931	0.4581
1	3	3	-7.8922	0.0582	1	1	6	-24.6062	0.4929
3	3	1	6.0889	0.0382	3	5	0	12.5165	0.1707
0	2	4	-40.5739	0.2268	2	4	4	-53.0252	0.2220
4	2	0	-44.2051	0.2641	4	4	2	52.8242	0.2088
4	2	1	91.5610	0.2197	1	5	3	43.3460	0.1356
0	4	2	65.0569	0.2455	3	5	1	-43.9334	0.1291
2	4	0	-67.3358	0.2498	5	3	2	45.2077	0.1210
3	3	2	54.3261	0.2120	2	0	6	-76.5039	0.2270
2	4	1	-73.8666	0.1937	6	0	2	-75.7109	0.3013
2	2	4	-38.0758	0.2405	0	2	6	31.1174	0.3915

FullProf refinement **FP1**									
h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	40.7345	0.2096	4	2	2	37.5804	0.2370
1	1	1	64.5052	0.0873	3	1	4	26.7235	0.3336
0	0	2	-143.4170	0.0941	5	1	0	28.7526	0.3406
2	0	0	143.4150	0.0939	2	4	2	63.4189	0.2160
0	2	0	-56.6760	0.2481	1	1	5	45.0958	0.1213
0	2	1	126.2070	0.1331	5	1	1	44.5522	0.1468
1	1	2	-39.0491	0.1376	1	3	4	-50.6649	0.2222
2	0	2	-121.7720	0.1930	0	4	3	70.2948	0.3797
0	2	2	46.7315	0.1206	3	3	3	-6.5787	0.2953
2	2	0	-58.1232	0.1493	0	2	5	81.2804	0.2300
2	2	1	115.1760	0.1047	4	2	3	-82.0426	0.2157
3	1	0	28.7209	0.2764	5	1	2	-28.6295	0.2858
1	1	3	-49.6163	0.0997	1	5	0	15.0741	0.4152
3	1	1	53.4831	0.1038	1	5	1	-48.1821	0.2507
1	3	0	-59.5594	0.2434	2	4	3	64.9802	0.1889
1	3	1	7.3136	0.0535	4	0	4	85.7874	0.2734
2	2	2	48.4180	0.2010	2	2	5	76.8323	0.3256
0	2	3	-108.7440	0.2299	1	5	2	-16.0008	0.2060
3	1	2	-30.0424	0.2404	0	4	4	-55.3191	0.2499
1	3	2	59.7728	0.1737	4	4	0	-55.7238	0.2170
0	0	4	113.2170	0.2317	3	1	5	39.9921	0.1477
4	0	0	113.3210	0.2622	5	1	3	-38.5552	0.1546
2	2	3	-99.6677	0.1767	3	3	4	-48.2457	0.1675
1	1	4	31.4695	0.2301	5	3	0	-46.0810	0.1430
0	4	0	-70.8429	0.4208	0	0	6	-85.2388	0.2129
3	1	3	-44.7739	0.2028	4	4	1	-61.6115	0.1638
3	3	0	-57.9366	0.2166	6	0	0	85.0594	0.2818
0	4	1	-74.7562	0.0978	1	3	5	5.5785	0.0753
2	0	4	101.4610	0.1309	5	3	1	5.8047	0.0783
4	0	2	-101.7240	0.1457	4	2	4	-31.6043	0.4385
1	3	3	-7.9289	0.0617	1	1	6	-25.2655	0.4724
3	3	1	6.1573	0.0405	3	5	0	12.5654	0.1635
0	2	4	-40.1529	0.2352	2	4	4	-53.6051	0.2211
4	2	0	-43.7076	0.2744	4	4	2	53.3815	0.2082
4	2	1	92.1824	0.2199	1	5	3	43.8248	0.1352
0	4	2	66.4644	0.2398	3	5	1	-44.4237	0.1288
2	4	0	-68.7571	0.2441	5	3	2	45.6861	0.1210
3	3	2	55.3501	0.2084	2	0	6	-77.1912	0.2263
2	4	1	-74.6997	0.1915	6	0	2	-76.4283	0.2986
2	2	4	-38.3912	0.2394	0	2	6	31.4719	0.3791

FullProf refinement **FP3**									
h	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	*h*	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	40.5869	0.1417	4	2	2	37.5669	0.3209
1	1	1	64.5525	0.0964	3	1	4	26.7732	0.4975
0	0	2	-144.3150	0.1003	5	1	0	28.9182	0.4744
2	0	0	144.1960	0.0998	2	4	2	63.0943	0.2506
0	2	0	-55.7337	0.4258	1	1	5	44.9080	0.1308
0	2	1	126.9690	0.1410	5	1	1	44.2901	0.1605
1	1	2	-39.0008	0.2141	1	3	4	-50.4232	0.2504
2	0	2	-121.5480	0.2413	0	4	3	69.7331	0.5012
0	2	2	46.4578	0.1629	3	3	3	-6.7250	0.8276
2	2	0	-57.8609	0.2023	0	2	5	80.9380	0.2683
2	2	1	115.1170	0.1099	4	2	3	-81.6192	0.2399
3	1	0	28.0732	0.5257	5	1	2	-28.7137	0.3846
1	1	3	-49.5571	0.1234	1	5	0	15.7528	0.8241
3	1	1	53.3869	0.1206	1	5	1	-47.7638	0.3286
1	3	0	-59.4667	0.3350	2	4	3	64.6737	0.2163
1	3	1	7.2077	0.0775	4	0	4	85.3112	0.3262
2	2	2	48.1770	0.2685	2	2	5	76.3263	0.4080
0	2	3	-108.4420	0.2544	1	5	2	-16.2911	0.2984
3	1	2	-30.4625	0.3540	0	4	4	-55.2343	0.2996
1	3	2	59.8394	0.2283	4	4	0	-55.6202	0.2549
0	0	4	112.8230	0.2592	3	1	5	39.6945	0.1669
4	0	0	113.1400	0.3291	5	1	3	-38.1972	0.1749
2	2	3	-99.1778	0.2066	3	3	4	-47.8155	0.1866
1	1	4	31.8141	0.3296	5	3	0	-45.7141	0.1583
0	4	0	-70.6760	0.5921	0	0	6	-85.0081	0.2326
3	1	3	-44.6239	0.2483	4	4	1	-61.4633	0.1810
3	3	0	-58.0661	0.2700	6	0	0	84.8009	0.3196
0	4	1	-74.4599	0.1034	1	3	5	5.4577	0.1043
2	0	4	101.0120	0.1393	5	3	1	5.6925	0.1142
4	0	2	-101.2950	0.1614	4	2	4	-31.2570	0.6704
1	3	3	-7.8986	0.0882	1	1	6	-25.2664	0.7623
3	3	1	6.1125	0.0561	3	5	0	12.3195	0.2253
0	2	4	-40.1775	0.3210	2	4	4	-53.2901	0.2586
4	2	0	-43.5274	0.3947	4	4	2	53.0977	0.2395
4	2	1	91.8000	0.2627	1	5	3	43.4638	0.1492
0	4	2	66.0374	0.3039	3	5	1	-44.0923	0.1419
2	4	0	-68.4245	0.3050	5	3	2	45.4231	0.1320
3	3	2	55.4915	0.2430	2	0	6	-76.7006	0.2531
2	4	1	-75.4013	0.2121	6	0	2	-75.8654	0.3444
2	2	4	-38.3293	0.3107	0	2	6	31.9094	0.5057

FullProf refinement **FP4**

h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	40.8977	0.1740	4	2	2	38.9536	0.1937
1	1	1	64.4274	0.0812	3	1	4	27.3634	0.2629
0	0	2	-139.4670	0.0895	5	1	0	29.4805	0.2646
2	0	0	139.3440	0.0896	2	4	2	63.9716	0.1862
0	2	0	-56.5119	0.2221	1	1	5	45.0001	0.1079
0	2	1	126.8680	0.1200	5	1	1	44.1888	0.1265
1	1	2	-39.2597	0.1214	1	3	4	-50.2613	0.1857
2	0	2	-122.6190	0.1737	0	4	3	70.6050	0.3207
0	2	2	46.8020	0.1073	3	3	3	-7.2777	0.1572
2	2	0	-58.1185	0.1331	0	2	5	82.1561	0.2072
2	2	1	115.6270	0.0938	4	2	3	-82.8633	0.1955
3	1	0	30.5444	0.1823	5	1	2	-28.1746	0.2162
1	1	3	-49.8046	0.0891	1	5	0	15.1867	0.2430
3	1	1	53.6514	0.0924	1	5	1	-47.7588	0.2055
1	3	0	-59.6575	0.2102	2	4	3	65.4633	0.1703
1	3	1	7.5590	0.0417	4	0	4	86.5246	0.2408
2	2	2	48.5544	0.1800	2	2	5	78.3358	0.2795
0	2	3	-109.4480	0.2072	1	5	2	-15.6677	0.1358
3	1	2	-30.0378	0.2000	0	4	4	-56.0480	0.2116
1	3	2	59.4315	0.1520	4	4	0	-56.4329	0.1851
0	0	4	114.0010	0.2056	3	1	5	40.0464	0.1255
4	0	0	114.2640	0.2327	5	1	3	-38.4907	0.1299
2	2	3	-100.3180	0.1590	3	3	4	-47.6251	0.1413
1	1	4	31.5176	0.1725	5	3	0	-45.6263	0.1220
0	4	0	-70.9966	0.3375	0	0	6	-85.4071	0.1952
3	1	3	-45.5096	0.1619	4	4	1	-61.5614	0.1493
3	3	0	-56.2458	0.1652	6	0	0	84.8037	0.2508
0	4	1	-75.3154	0.0884	1	3	5	5.7744	0.0568
2	0	4	102.3060	0.1191	5	3	1	6.0607	0.0599
4	0	2	-102.5440	0.1303	4	2	4	-32.4695	0.3255
1	3	3	-8.3554	0.0450	1	1	6	-26.5480	0.3232
3	3	1	6.5164	0.0310	3	5	0	12.4551	0.1070
0	2	4	-40.9854	0.1850	2	4	4	-54.1512	0.1937
4	2	0	-44.3110	0.2200	4	4	2	53.7882	0.1820
4	2	1	92.3198	0.1972	1	5	3	43.4346	0.1165
0	4	2	67.3806	0.2053	3	5	1	-44.0587	0.1114
2	4	0	-69.7224	0.2086	5	3	2	45.2715	0.1070
3	3	2	56.7024	0.1636	2	0	6	-77.8879	0.2007
2	4	1	-76.6990	0.1596	6	0	2	-76.9941	0.2595
2	2	4	-40.2273	0.1893	0	2	6	31.9199	0.2782

Jana2006 refinement **J1**									
h	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	*h*	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	40.7860	0.4196	4	2	2	37.2400	0.4329
1	1	1	64.4690	0.6547	3	1	4	26.2040	0.4457
0	0	2	-143.7500	1.4494	5	1	0	28.0150	0.4736
2	0	0	143.6300	1.4482	2	4	2	63.3140	0.6677
0	2	0	-58.6460	0.6283	1	1	5	44.6570	0.4729
0	2	1	127.1300	1.2844	5	1	1	44.4910	0.4737
1	1	2	-38.6400	0.4065	1	3	4	-50.7550	0.5705
2	0	2	-117.6000	1.1918	0	4	3	70.2330	0.8001
0	2	2	47.6690	0.4931	3	3	3	-6.1777	0.3146
2	2	0	-59.2590	0.6119	0	2	5	79.7120	0.8280
2	2	1	116.4600	1.1775	4	2	3	-80.7200	0.8383
3	1	0	28.1190	0.4150	5	1	2	-28.7640	0.3752
1	1	3	-49.6700	0.5112	1	5	0	14.8300	0.3886
3	1	1	53.5270	0.5502	1	5	1	-47.0360	0.5081
1	3	0	-60.7210	0.6649	2	4	3	64.4340	0.6761
1	3	1	7.1117	0.0769	4	0	4	85.0110	0.8932
2	2	2	48.7780	0.5201	2	2	5	75.5460	0.8252
0	2	3	-108.1800	1.1080	1	5	2	-15.8180	0.1998
3	1	2	-28.8520	0.3845	0	4	4	-53.4880	0.5877
1	3	2	59.4520	0.6275	4	4	0	-54.0700	0.5919
0	0	4	112.7000	1.1573	3	1	5	39.7740	0.4362
4	0	0	113.0300	1.1608	5	1	3	-38.5130	0.4229
2	2	3	-98.2510	1.0026	3	3	4	-48.3850	0.5171
1	1	4	30.7270	0.4012	5	3	0	-46.4200	0.4942
0	4	0	-69.7040	0.8047	0	0	6	-85.0380	0.8950
3	1	3	-44.5150	0.5038	4	4	1	-61.4690	0.6476
3	3	0	-56.1100	0.5953	6	0	0	84.9830	0.8984
0	4	1	-73.7060	0.7511	1	3	5	5.4036	0.0900
2	0	4	99.9650	1.0185	5	3	1	5.6110	0.0992
4	0	2	-100.0700	1.0196	4	2	4	-31.0540	0.5535
1	3	3	-7.9739	0.0981	1	1	6	-24.1340	0.6190
3	3	1	6.1192	0.0756	3	5	0	12.8350	0.1483
0	2	4	-40.3750	0.4922	2	4	4	-53.2900	0.5905
4	2	0	-44.0380	0.5369	4	4	2	52.9370	0.5860
4	2	1	92.0250	0.9491	1	5	3	43.2310	0.4616
0	4	2	67.7300	0.7277	3	5	1	-43.7820	0.4675
2	4	0	-69.8270	0.7499	5	3	2	44.8560	0.4778
3	3	2	56.0840	0.6032	2	0	6	-77.0280	0.8143
2	4	1	-75.9980	0.7979	6	0	2	-76.8870	0.8176
2	2	4	-38.4560	0.4469	0	2	6	31.2770	0.5230

Jana2006 refinement **J2**									
h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	40.8340	0.4200	4	2	2	37.4640	0.4350
1	1	1	64.4740	0.6548	3	1	4	26.1470	0.4450
0	0	2	-143.7600	1.4495	5	1	0	27.9730	0.4730
2	0	0	143.6600	1.4484	2	4	2	63.5720	0.6702
0	2	0	-57.9390	0.6217	1	1	5	44.6140	0.4723
0	2	1	127.0900	1.2841	5	1	1	44.4430	0.4731
1	1	2	-38.5590	0.4057	1	3	4	-50.6120	0.5691
2	0	2	-117.6500	1.1924	0	4	3	69.8110	0.7961
0	2	2	47.6490	0.4929	3	3	3	-6.0605	0.3186
2	2	0	-59.2850	0.6122	0	2	5	79.8750	0.8295
2	2	1	116.4500	1.1774	4	2	3	-80.8780	0.8397
3	1	0	28.6830	0.4171	5	1	2	-28.7010	0.3736
1	1	3	-49.6320	0.5108	1	5	0	14.5930	0.3840
3	1	1	53.4840	0.5498	1	5	1	-47.0590	0.5084
1	3	0	-60.7210	0.6650	2	4	3	64.3820	0.6755
1	3	1	7.1455	0.0774	4	0	4	85.1570	0.8947
2	2	2	48.4700	0.5173	2	2	5	75.5450	0.8250
0	2	3	-108.8300	1.1144	1	5	2	-15.7080	0.1980
3	1	2	-29.1950	0.3866	0	4	4	-53.6840	0.5896
1	3	2	59.5970	0.6288	4	4	0	-54.2680	0.5939
0	0	4	113.1300	1.1615	3	1	5	39.7160	0.4354
4	0	0	113.4800	1.1652	5	1	3	-38.4530	0.4215
2	2	3	-98.3950	1.0040	3	3	4	-48.3660	0.5169
1	1	4	31.1880	0.4039	5	3	0	-46.3990	0.4939
0	4	0	-69.3040	0.8012	0	0	6	-85.1730	0.8963
3	1	3	-44.1970	0.5007	4	4	1	-61.4100	0.6470
3	3	0	-56.0510	0.5947	6	0	0	85.1130	0.8997
0	4	1	-73.5930	0.7500	1	3	5	5.4828	0.0869
2	0	4	100.0700	1.0196	5	3	1	5.6541	0.0998
4	0	2	-100.1800	1.0207	4	2	4	-31.0030	0.5516
1	3	3	-8.0536	0.0990	1	1	6	-24.6080	0.6158
3	3	1	6.1882	0.0764	3	5	0	12.7630	0.1471
0	2	4	-40.3220	0.4907	2	4	4	-53.5210	0.5923
4	2	0	-43.9120	0.5357	4	4	2	53.1660	0.5878
4	2	1	92.2290	0.9511	1	5	3	43.2300	0.4615
0	4	2	67.7490	0.7275	3	5	1	-43.7820	0.4675
2	4	0	-69.8450	0.7498	5	3	2	44.8140	0.4773
3	3	2	55.9660	0.6021	2	0	6	-77.0980	0.8150
2	4	1	-75.7730	0.7958	6	0	2	-76.9360	0.8180
2	2	4	-38.6760	0.4489	0	2	6	31.0300	0.5193

Jana2006 refinement **J3**

h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	40.7840	0.4195	4	2	2	37.4880	0.4349
1	1	1	64.4920	0.6549	3	1	4	26.1880	0.4440
0	0	2	-143.7900	1.4497	5	1	0	28.0170	0.4719
2	0	0	143.6800	1.4486	2	4	2	63.5550	0.6698
0	2	0	-58.2410	0.6244	1	1	5	44.6520	0.4727
0	2	1	127.0600	1.2838	5	1	1	44.4730	0.4733
1	1	2	-38.5390	0.4055	1	3	4	-50.6060	0.5686
2	0	2	-117.6500	1.1923	0	4	3	69.8680	0.7960
0	2	2	47.6890	0.4933	3	3	3	-6.0526	0.3073
2	2	0	-59.3200	0.6125	0	2	5	79.9470	0.8302
2	2	1	116.4600	1.1775	4	2	3	-80.9450	0.8404
3	1	0	28.7850	0.4162	5	1	2	-28.6900	0.3725
1	1	3	-49.6510	0.5110	1	5	0	14.7710	0.3824
3	1	1	53.5010	0.5499	1	5	1	-47.0550	0.5082
1	3	0	-60.7510	0.6650	2	4	3	64.4750	0.6763
1	3	1	7.0388	0.0762	4	0	4	85.2080	0.8951
2	2	2	48.4900	0.5174	2	2	5	75.6410	0.8258
0	2	3	-108.8300	1.1144	1	5	2	-15.8480	0.1932
3	1	2	-29.1850	0.3860	0	4	4	-53.6570	0.5891
1	3	2	59.5810	0.6285	4	4	0	-54.2380	0.5933
0	0	4	113.0000	1.1600	3	1	5	39.7440	0.4355
4	0	0	113.4900	1.1652	5	1	3	-38.5160	0.4209
2	2	3	-98.4550	1.0046	3	3	4	-48.3640	0.5167
1	1	4	31.2120	0.4027	5	3	0	-46.4000	0.4938
0	4	0	-69.3670	0.8010	0	0	6	-85.1590	0.8960
3	1	3	-44.2720	0.5011	4	4	1	-61.4500	0.6473
3	3	0	-56.0590	0.5945	6	0	0	85.1090	0.8995
0	4	1	-73.6680	0.7507	1	3	5	5.4141	0.0854
2	0	4	100.1000	1.0198	5	3	1	5.5882	0.0980
4	0	2	-100.2100	1.0210	4	2	4	-31.0470	0.5485
1	3	3	-7.9667	0.0977	1	1	6	-24.6370	0.6099
3	3	1	6.1012	0.0752	3	5	0	12.8920	0.1486
0	2	4	-40.3950	0.4907	2	4	4	-53.5220	0.5921
4	2	0	-43.9900	0.5357	4	4	2	53.1650	0.5875
4	2	1	92.2780	0.9516	1	5	3	43.2170	0.4613
0	4	2	67.7680	0.7276	3	5	1	-43.7080	0.4658
2	4	0	-69.8640	0.7499	5	3	2	44.8420	0.4775
3	3	2	55.9500	0.6018	2	0	6	-77.1250	0.8151
2	4	1	-75.7810	0.7957	6	0	2	-76.9660	0.8182
2	2	4	-38.6950	0.4488	0	2	6	31.0300	0.5159

GSAS+EXPGUI refinement **G1**									
h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	h	k	l	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	41.6422	0.5164	4	2	2	36.0935	0.4824
1	1	1	66.0401	0.8086	3	1	4	25.6471	0.3409
0	0	2	-146.9310	1.8319	5	1	0	29.6250	0.3651
2	0	0	146.5440	1.8284	2	4	2	65.4666	0.8256
0	2	0	-57.7864	0.6883	1	1	5	45.7053	0.5614
0	2	1	128.1530	1.5777	5	1	1	45.1058	0.5555
1	1	2	-40.6401	0.5018	1	3	4	-51.4004	0.6381
2	0	2	-122.2420	1.5727	0	4	3	73.1781	0.8668
0	2	2	38.7027	0.5702	3	3	3	-8.0422	0.0962
2	2	0	-60.3087	0.7134	0	2	5	81.4907	1.0447
2	2	1	116.6900	1.4349	4	2	3	-83.2824	1.0585
3	1	0	24.7756	0.3757	5	1	2	-29.2000	0.3572
1	1	3	-47.0496	0.6281	1	5	0	12.8219	0.1680
3	1	1	54.9027	0.6776	1	5	1	-49.0953	0.5969
1	3	0	-58.6331	0.7246	2	4	3	66.4790	0.8259
1	3	1	8.3144	0.1046	4	0	4	86.9136	1.1051
2	2	2	49.3259	0.6020	2	2	5	77.2226	0.9856
0	2	3	-108.8630	1.3775	1	5	2	-15.6264	0.1807
3	1	2	-29.9351	0.3838	0	4	4	-56.4753	0.7166
1	3	2	61.1833	0.7405	4	4	0	-57.6430	0.7258
0	0	4	115.6720	1.4395	3	1	5	40.4300	0.5133
4	0	0	115.7060	1.4408	5	1	3	-37.8254	0.4959
2	2	3	-101.8180	1.2744	3	3	4	-49.1369	0.6040
1	1	4	31.9101	0.4021	5	3	0	-44.5258	0.5726
0	4	0	-72.2725	0.8903	0	0	6	-88.4871	1.0718
3	1	3	-43.9569	0.5734	4	4	1	-61.7537	0.7632
3	3	0	-57.5690	0.7014	6	0	0	88.1310	1.0690
0	4	1	-73.9489	0.9483	1	3	5	6.0609	0.0833
2	0	4	101.7890	1.3028	5	3	1	6.5111	0.0867
4	0	2	-102.2110	1.3051	4	2	4	-31.7105	0.4142
1	3	3	-9.6229	0.1132	1	1	6	-24.8454	0.3173
3	3	1	6.1570	0.0898	3	5	0	9.7759	0.1447
0	2	4	-37.2220	0.4943	2	4	4	-54.9224	0.6965
4	2	0	-44.2933	0.5404	4	4	2	54.4547	0.6914
4	2	1	92.6863	1.1745	1	5	3	44.0188	0.5504
0	4	2	67.4519	0.8453	3	5	1	-45.1800	0.5578
2	4	0	-71.8896	0.8729	5	3	2	45.4100	0.5666
3	3	2	57.1296	0.6993	2	0	6	-79.2478	1.0003
2	4	1	-75.6164	0.9046	6	0	2	-78.4063	0.9988
2	2	4	-38.2966	0.5002	0	2	6	31.8645	0.3912

GSAS+EXPGUI refinement **G2**									
h	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$	*h*	*k*	*l*	$F_{obs}(\boldsymbol{H})$	$\sigma_{obs}(\boldsymbol{H})$
1	1	0	42.1719	0.5149	4	2	2	37.7443	0.4884
1	1	1	65.7365	0.8112	3	1	4	26.2971	0.3429
0	0	2	-147.5280	1.8323	5	1	0	30.2340	0.3671
2	0	0	147.3380	1.8289	2	4	2	65.2266	0.8204
0	2	0	-60.5386	0.6952	1	1	5	46.0688	0.5675
0	2	1	125.3780	1.5759	5	1	1	45.4047	0.5617
1	1	2	-39.5618	0.5013	1	3	4	-51.6232	0.6451
2	0	2	-124.9110	1.5741	3	3	3	-7.7525	0.0928
0	2	2	38.1392	0.5770	0	4	3	73.4852	0.8760
2	2	0	-59.0484	0.7202	0	2	5	81.3585	1.0467
2	2	1	115.2070	1.4342	4	2	3	-83.1565	1.0606
3	1	0	24.7637	0.3759	5	1	2	-29.4300	0.3597
1	1	3	-48.0420	0.6317	1	5	0	13.5150	0.1768
3	1	1	55.9886	0.6813	1	5	1	-48.9942	0.6017
1	3	0	-60.8239	0.7284	2	4	3	66.5501	0.8351
1	3	1	7.8856	0.1003	4	0	4	86.3795	1.1095
2	2	2	49.4361	0.6086	2	2	5	76.7069	0.9878
0	2	3	-107.7290	1.3773	1	5	2	-16.1120	0.1890
3	1	2	-28.4468	0.3849	0	4	4	-56.0469	0.7131
1	3	2	60.9950	0.7455	4	4	0	-57.2282	0.7223
0	0	4	115.3160	1.4421	3	1	5	40.8714	0.5201
4	0	0	115.3330	1.4437	5	1	3	-38.2760	0.5027
2	2	3	-101.9060	1.2743	3	3	4	-49.7760	0.6118
1	1	4	32.0166	0.4032	5	3	0	-45.1657	0.5805
0	4	0	-72.7103	0.8844	0	0	6	-89.0776	1.0764
3	1	3	-44.7256	0.5785	4	4	1	-62.7554	0.7724
3	3	0	-59.0002	0.7070	6	0	0	89.0740	1.0736
0	4	1	-74.9969	0.9577	1	3	5	6.1425	0.0804
2	0	4	102.4130	1.3060	5	3	1	6.6414	0.0835
4	0	2	-102.9210	1.3082	4	2	4	-34.0377	0.4198
1	3	3	-9.2994	0.1092	1	1	6	-26.2962	0.3200
3	3	1	5.8102	0.0859	3	5	0	10.5831	0.1528
0	2	4	-37.3858	0.5005	2	4	4	-54.9082	0.6934
4	2	0	-44.0692	0.5466	4	4	2	54.3806	0.6884
4	2	1	90.5568	1.1752	1	5	3	43.8644	0.5561
0	4	2	65.7693	0.8401	3	5	1	-45.0001	0.5636
2	4	0	-70.1939	0.8675	0	2	6	31.3570	0.3972
3	3	2	57.1410	0.7057	5	3	2	45.4123	0.5750
2	4	1	-76.6009	0.9137	6	2	0	-31.2426	0.3993
2	2	4	-40.0462	0.5061	2	0	6	-78.4055	1.0052