**Supplement for the article: PDF analysis of ferrihydrite: Critical assessment of the underconstrained akdalaite model**

Figure S1. Structure of the akdalaite model and its parametrization in PDFgui

Polyhedral representation of the akdalaite unit cell. Independent atoms in the asymmetric unit are labeled.	Screen shot of the PDFgui interface window showing the parametrization of the akdalaite model. Symmetry-related positions in the full cell were generated from the asymmetric unit and symmetry constraints of the $P6_3mc$ space group.	Screen shot of the initial and refined parameter values. The Fe1 site occupancy was fixed to 1.0 to reduce correlations (19 parameters adjusted).

Phase Constraints

| a | @4 | b | @4 | c | @5 |
| alpha | | beta | | gamma | |
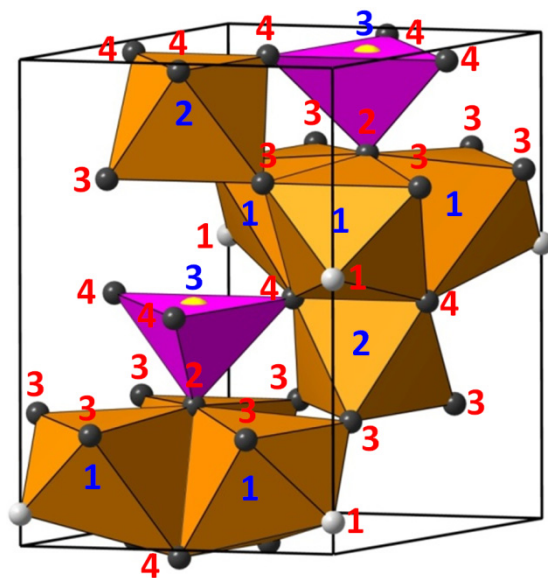
Scale Factor

delta1 @6   delta2   spdiameter @8

sratio

Included Pairs: all-all

	elem		x	y	z	u11	u22	u33	u12	u13	u23	occ
1	Fe	1	@11	-@11 +1	@12	@100	@100	@100				@301
2	Fe	1	@11	+2*@11	@12	@100	@100	@100				@301
3	Fe	1	-2*@11 +1	-@11 +1	@12	@100	@100	@100				@301
4	Fe	1	-@11 +1	@11	@12 -0.5	@100	@100	@100				@301
5	Fe	1	-@11 +1	-2*@11 +1	@12 -0.5	@100	@100	@100				@301
6	Fe	1	+2*@11	@11	@12 -0.5	@100	@100	@100				@301
7	Fe	2			@13	@100	@100	@100				@302
8	Fe	2			@13 +0.5	@100	@100	@100				@302
9	Fe	3			@15	@100	@100	@100				@303
10	Fe	3			@15 -0.5	@100	@100	@100				@303
11	O	1			@16	@200	@200	@200				
12	O	1			@16 +0.5	@200	@200	@200				
13	O	2			@17	@200	@200	@200				
14	O	2			@17 +0.5	@200	@200	@200				
15	O	3	@18	-@18 +1	@19	@200	@200	@200				
16	O	3	@18	+2*@18	@19	@200	@200	@200				
17	O	3	-2*@18 +1	-@18 +1	@19	@200	@200	@200				
18	O	3	-@18 +1	@18	@19 +0.5	@200	@200	@200				
19	O	3	-@18 +1	-2*@18 +1	@19 +0.5	@200	@200	@200				
20	O	3	+2*@18	@18	@19 +0.5	@200	@200	@200				
21	O	4	@20	-@20 +1	@21	@200	@200	@200				
22	O	4	@20	+2*@20 -1	@21	@200	@200	@200				
23	O	4	-2*@20 +2	-@20 +1	@21	@200	@200	@200				
24	O	4	-@20 +1	@20	@21 -0.5	@200	@200	@200				
25	O	4	-@20 +1	-2*@20 +2	@21 -0.5	@200	@200	@200				
26	O	4	+2*@20 -1	@20	@21 -0.5	@200	@200	@200				

		Initial	Fixed	Refined
@	1	1.3		1.26078215171
@	2	0.137		0.0735800893587
@	4	5.928		5.94375215241
@	5	9.126		9.16963651216
@	6	1.8		1.88517177714
@	8	35.0	☑	35.0
@	11	0.1695		0.16918043634
@	12	0.6365		0.63630493601
@	13	0.3379		0.331055495526
@	15	0.9595		0.953356338802
@	16	0.0446		0.0659270295649
@	17	0.7634		0.769203681119
@	18	0.1697		0.167758743399
@	19	0.2467		0.244748555132
@	20	0.5227		0.523994536215
@	21	0.9796		0.980284557646
@100		0.011		0.0117534396498
@200		0.007		0.00384039869658
@301		1.0	☑	1.0
@302		0.97		0.855348533147
@303		0.96		0.861677349147

@1 is the scale factor and @2 is the resolution dampening (Q_{damp}). Q_{broad} was fixed to 0.069 Å^{-1}. Full results are listed in Table S2.

Figure S2. Structure of the modified akdalaite model and its parametrization in PDFgui

| Polyhedral representation of the modified akdalaite unit cell. Independent atoms in the asymmetric unit are labeled. The oxgen atoms and hydroxyls are positioned as in the f-phase (Fig. 1). | Screen shot of the PDFgui interface window showing the parametrization of the modified akdalaite model. | Screen shot of the initial and refined parameter values. |
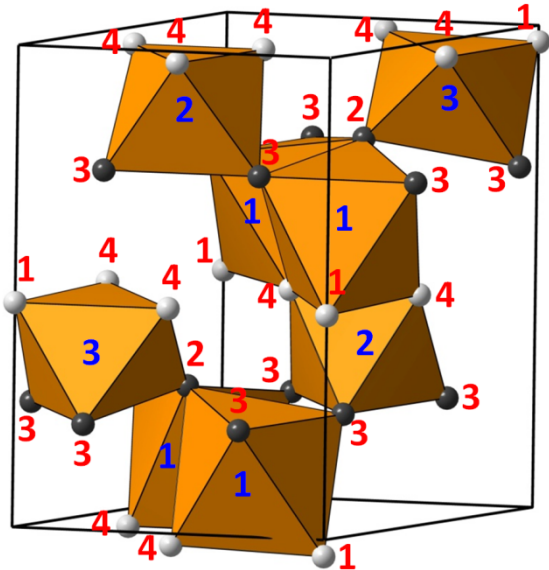
Phase Constraints

a @4   b @4   c @5
alpha   beta   gamma

Scale Factor
delta1   delta2   spdiameter @8
sratio @6

Included Pairs   all-all

	elem		x	y	z	u11	u22	u33	u12	u13	u23	occ
1	Fe	1	@11	+2*@11	@12	@100	@100	@100				@301
2	Fe	1	-2*@11 +1	-@11 +1	@12	@100	@100	@100				@301
3	Fe	1	-@11 +1	-2*@11 +1	@12 -0.5	@100	@100	@100				@301
4	Fe	1	+2*@11	@11	@12 -0.5	@100	@100	@100				@301
5	Fe	2			@13	@100	@100	@100				@302
6	Fe	2			@13 +0.5	@100	@100	@100				@302
7	Fe	3	@14	-@14 +1	@15	@100	@100	@100				@303
8	Fe	3	-@14 +1	@14	@15 -0.5	@100	@100	@100				@303
9	O	1			@16	@200	@200	@200				
10	O	1			@16 +0.5	@200	@200	@200				
11	O	2			@17	@200	@200	@200				
12	O	2			@17 +0.5	@200	@200	@200				
13	O	3	@18	-@18 +1	@19	@200	@200	@200				
14	O	3	@18	+2*@18	@19	@200	@200	@200				
15	O	3	-2*@18 +1	-@18 +1	@19	@200	@200	@200				
16	O	3	-@18 +1	@18	@19 +0.5	@200	@200	@200				
17	O	3	-@18 +1	-2*@18 +1	@19 +0.5	@200	@200	@200				
18	O	3	+2*@18	@18	@19 +0.5	@200	@200	@200				
19	O	4	@20	-@20 +1	@21	@200	@200	@200				
20	O	4	@20	+2*@20 -1	@21	@200	@200	@200				
21	O	4	-2*@20 +2	-@20 +1	@21	@200	@200	@200				
22	O	4	-@20 +1	@20	@21 -0.5	@200	@200	@200				
23	O	4	-@20 +1	-2*@20 +2	@21 -0.5	@200	@200	@200				
24	O	4	+2*@20 -1	@20	@21 -0.5	@200	@200	@200				

		Initial	Fixed	Refined
@	1	1.3		1.46023322482
@	2	0.137		0.0797513125045
@	4	5.928		5.95041595549
@	5	9.126		9.13279706467
@	6	1.0		0.461806863636
@	8	35.0	☑	35.0
@	11	0.1695		0.17491586752
@	12	0.6365	☑	0.6365
@	13	0.3379		0.320720779344
@	14	0.1697		0.169786935837
@	15	0.85		0.842817540034
@	16	-0.0446		-0.0344265657565
@	17	0.7634		0.779493448447
@	18	0.1697		0.167311652982
@	19	0.2467		0.233612214827
@	20	0.5227		0.528761606496
@	21	0.9796		0.971194873621
@	100	0.011		0.00697294046269
@	200	0.007		0.00563328878938
@	301	1.0	☑	1.0
@	302	0.97		1.05785376365
@	303	0.96		0.83144015261

The z(Fe1) position was fixed during the refinement to the value of Michel et al. (2007) to limit the total number of fitted parameters to 19. Full results are listed in Table S3.

Table S1. Results from the akdalaite fit to the 6Fh PDF with 20 adjusted parameters

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* Mon Mar 25 09:17:47 2013

 ====================================================================================
 PDF REFINEMENT
    Using PDFFIT version : 1.0-r6773-20111122
 ====================================================================================
 ------------------------------------------------------------------------------------
 PHASE 1 : UNNAMED
 ------------------------------------------------------------------------------------
 Scale factor            : 1
    Particle diameter    : 35 A
    Step cutoff          : not applied
 Quad. corr. factor      : 0
 Lin. corr. factor       : 1.81458 (0.21)
 Low r sigma ratio       : 1
 R cutoff [A]            : 0
 Lattice parameters      : 5.9395 (0.0092)      5.9395 (0.0092)      9.17173 (0.025)
            & angles      : 90                  90                   120

 Atom positions & occupancies :
    FE    0.170377 (0.001)     0.829623 (0.001)     0.638305 (2.2e+04)   0.82616 (0.076)
    FE    0.170377 (0.001)     0.340754 (0.002)     0.638305 (2.2e+04)   0.82616 (0.076)
    FE    0.659246 (0.002)     0.829623 (0.001)     0.638305 (2.2e+04)   0.82616 (0.076)
    FE    0.829623 (0.001)     0.170377 (0.001)     0.138305 (2.2e+04)   0.82616 (0.076)
    FE    0.829623 (0.001)     0.659246 (0.002)     0.138305 (2.2e+04)   0.82616 (0.076)
    FE    0.340754 (0.002)     0.170377 (0.001)     0.138305 (2.2e+04)   0.82616 (0.076)
    FE    0.333333             0.666667             0.334625 (2.2e+04)   0.736728 (0.18)
    FE    0.666667             0.333333             0.834625 (2.2e+04)   0.736728 (0.18)
    FE    0.333333             0.666667             0.953882 (2.2e+04)   0.815759 (0.14)
    FE    0.666667             0.333333             0.453882 (2.2e+04)   0.815759 (0.14)
    O     0                    0                    0.0612022 (2.2e+04)  1
    O     0                    0                    0.561202 (2.2e+04)   1
    O     0.333333             0.666667             0.757992 (2.2e+04)   1
    O     0.666667             0.333333             0.257992 (2.2e+04)   1
    O     0.171725 (0.0041)    0.828275 (0.0041)    0.246359 (2.2e+04)   1
    O     0.171725 (0.0041)    0.343449 (0.0082)    0.246359 (2.2e+04)   1
    O     0.656551 (0.0082)    0.828275 (0.0041)    0.246359 (2.2e+04)   1
    O     0.828275 (0.0041)    0.171725 (0.0041)    0.746359 (2.2e+04)   1
    O     0.828275 (0.0041)    0.656551 (0.0082)    0.746359 (2.2e+04)   1
    O     0.343449 (0.0082)    0.171725 (0.0041)    0.746359 (2.2e+04)   1
    O     0.519454 (0.0035)    0.480546 (0.0035)    0.977773 (2.2e+04)   1
    O     0.519454 (0.0035)    0.0389082 (0.0071)   0.977773 (2.2e+04)   1
    O     0.961092 (0.0071)    0.480546 (0.0035)    0.977773 (2.2e+04)   1
    O     0.480546 (0.0035)    0.519454 (0.0035)    0.477773 (2.2e+04)   1
    O     0.480546 (0.0035)    0.961092 (0.0071)    0.477773 (2.2e+04)   1
    O     0.0389082 (0.0071)   0.519454 (0.0035)    0.477773 (2.2e+04)   1

 Anisotropic temperature factors :
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    FE    0.0105771 (0.0011)   0.0105771 (0.0011)   0.0105771 (0.0011)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
    O     0.0105045 (0.0024)   0.0105045 (0.0024)   0.0105045 (0.0024)
```

```
------------------------------------------------------------------------
DATA SET : 1 (string)
------------------------------------------------------------------------
Data range in r [A]     : 1.38      -> 20          Step dr  : 0.02
Calculated range        : 1.38      -> 21.7952
Refinement r range      : 1.38      -> 20          Data pts : 0      -> 931
Reduced chi squared     : 0.222497
Rw - value              : 0.297642


Experimental settings   :
  Radiation             : X-Rays
  Termination at Qmax   : 21 A**-1
  DQ dampening Qdamp     : 0.0727986 (0.007) A**-1
  DQ broadening Qbroad  : 0.069 A**-1
  Scale factor          : 1.37253 (0.089)

Selected phases and atoms for this data set :
  Phase 1 :
    Atoms (i) :   FE   O
    Atoms (j) :   FE   O

Relative phase content in terms of
          atoms                     unit cells                mass
Phase 1 : 1                         1                         1


------------------------------------------------------------------------
PARAMETER INFORMATION :
------------------------------------------------------------------------
Number of constraints        : 157
Number of refined parameters : 20
Number of fixed parameters   : 1

Refinement parameters :
  1: 1.37253 (0.089)         2: 0.0727986 (0.007)      4: 5.9395 (0.0092)
  5: 9.17173 (0.025)         6: 1.81458 (0.21)         8: 35
 11: 0.170377 (0.001)       12: 0.638305 (2.2e+04)    13: 0.334625 (2.2e+04)
 15: 0.953882 (2.2e+04)     16: 0.0612022 (2.2e+04)   17: 0.757992 (2.2e+04)
 18: 0.171725 (0.0041)      19: 0.246359 (2.2e+04)    20: 0.519454 (0.0035)
 21: 0.977773 (2.2e+04)    100: 0.0105771 (0.0011)   200: 0.0105045 (0.0024)
301: 0.82616 (0.076)       302: 0.736728 (0.18)      303: 0.815759 (0.14)
------------------------------------------------------------------------
REFINEMENT INFORMATION:
------------------------------------------------------------------------
Number of iterations : 5
Reduced chi squared  : 0.204832
Rw - value           : 0.285582

Correlations greater than 0.8 :

  Corr(p[12], p[13]) = 1
  Corr(p[12], p[15]) = 1
  Corr(p[12], p[16]) = 1
  Corr(p[12], p[17]) = 1
  Corr(p[12], p[19]) = 1
  Corr(p[12], p[21]) = 1
  Corr(p[13], p[15]) = 1
  Corr(p[13], p[16]) = 1
  Corr(p[13], p[17]) = 1
  Corr(p[13], p[19]) = 1
  Corr(p[13], p[21]) = 1
  Corr(p[15], p[16]) = 1
  Corr(p[15], p[17]) = 1
  Corr(p[15], p[19]) = 1
  Corr(p[15], p[21]) = 1
  Corr(p[16], p[17]) = 1
  Corr(p[16], p[19]) = 1
  Corr(p[16], p[21]) = 1
  Corr(p[17], p[19]) = 1
  Corr(p[17], p[21]) = 1
  Corr(p[19], p[21]) = 1
  Corr(p[302], p[303]) = -0.823727
========================================================================
```

Table S2. Results from the akdalaite fit to the 6Fh PDF with 19 adjusted parameters

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* Mon Mar 25 09:19:53 2013

=================================================================================
PDF REFINEMENT
   Using PDFFIT version : 1.0-r6773-20111122
=================================================================================
---------------------------------------------------------------------------------
PHASE 1 : UNNAMED
---------------------------------------------------------------------------------
Scale factor            : 1
  Particle diameter     : 35 A
  Step cutoff           : not applied
Quad. corr. factor      : 0
Lin. corr. factor       : 1.88517 (0.0072)
Low r sigma ratio       : 1
R cutoff [A]            : 0
Lattice parameters      : 5.94375 (0.0083)    5.94375 (0.0083)     9.16964 (0.023)
          & angles      : 90                  90                   120

Atom positions & occupancies :
  FE    0.16918 (0.0011)    0.83082 (0.0011)    0.636305            1
  FE    0.16918 (0.0011)    0.338361 (0.0022)   0.636305            1
  FE    0.661639 (0.0022)   0.83082 (0.0011)    0.636305            1
  FE    0.83082 (0.0011)    0.16918 (0.0011)    0.136305            1
  FE    0.83082 (0.0011)    0.661639 (0.0022)   0.136305            1
  FE    0.338361 (0.0022)   0.16918 (0.0011)    0.136305            1
  FE    0.333333           0.666667             0.331055            0.855349 (0.2)
  FE    0.666667           0.333333             0.831055            0.855349 (0.2)
  FE    0.333333           0.666667             0.953356            0.861677 (0.15)
  FE    0.666667           0.333333             0.453356            0.861677 (0.15)
  O     0                  0                    0.065927            1
  O     0                  0                    0.565927            1
  O     0.333333           0.666667             0.769204            1
  O     0.666667           0.333333             0.269204            1
  O     0.167759 (0.0027)   0.832241 (0.0027)   0.244749            1
  O     0.167759 (0.0027)   0.335517 (0.0055)   0.244749            1
  O     0.664483 (0.0055)   0.832241 (0.0027)   0.244749            1
  O     0.832241 (0.0027)   0.167759 (0.0027)   0.744749            1
  O     0.832241 (0.0027)   0.664483 (0.0055)   0.744749            1
  O     0.335517 (0.0055)   0.167759 (0.0027)   0.744749            1
  O     0.523995 (0.003)    0.476005 (0.003)    0.980285            1
  O     0.523995 (0.003)    0.0479891 (0.0059)  0.980285            1
  O     0.952011 (0.0059)   0.476005 (0.003)    0.980285            1
  O     0.476005 (0.003)    0.523995 (0.003)    0.480285            1
  O     0.476005 (0.003)    0.952011 (0.0059)   0.480285            1
  O     0.0479891 (0.0059)  0.523995 (0.003)    0.480285            1

Anisotropic temperature factors :
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  FE    0.0117534 (0.0011)  0.0117534 (0.0011)  0.0117534 (0.0011)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
  O     0.0038404 (0.0016)  0.0038404 (0.0016)  0.0038404 (0.0016)
```

```
--------------------------------------------------------------------------------
DATA SET : 1 (string)
--------------------------------------------------------------------------------
Data range in r [A]    : 1.38      -> 20           Step dr  : 0.02
Calculated range       : 1.38      -> 21.7952
Refinement r range     : 1.38      -> 20           Data pts : 0      -> 931
Reduced chi squared    : 0.183335
Rw - value             : 0.270329


Experimental settings  :
  Radiation            : X-Rays
  Termination at Qmax  : 21 A**-1
  DQ dampening Qdamp    : 0.0735801 (0.0062) A**-1
  DQ broadening Qbroad  : 0.069 A**-1
  Scale factor         : 1.26078 (0.048)

Selected phases and atoms for this data set :
  Phase 1 :
    Atoms (i) :   FE   O
    Atoms (j) :   FE   O

Relative phase content in terms of
          atoms                      unit cells              mass
Phase 1 : 1                          1                       1


--------------------------------------------------------------------------------
PARAMETER INFORMATION :
--------------------------------------------------------------------------------
Number of constraints      : 157
Number of refined parameters : 19
Number of fixed parameters   : 2

Refinement parameters :
  1: 1.26078 (0.048)        2: 0.0735801 (0.0062)     4: 5.94375 (0.0083)
  5: 9.16964 (0.023)        6: 1.88517 (0.0072)       8: 35
 11: 0.16918 (0.0011)      12: 0.636305              13: 0.331055
 15: 0.953356              16: 0.065927              17: 0.769204
 18: 0.167759 (0.0027)     19: 0.244749              20: 0.523995 (0.003)
 21: 0.980285             100: 0.0117534 (0.0011)   200: 0.0038404 (0.0016)
301: 1                    302: 0.855349 (0.2)       303: 0.861677 (0.15)
--------------------------------------------------------------------------------
REFINEMENT INFORMATION:
--------------------------------------------------------------------------------
Number of iterations : 22
Reduced chi squared  : 0.182609
Rw - value           : 0.269793

Correlations greater than 0.8 :

  Corr(p[302], p[303]) = -0.866634
================================================================================
```

Table S3. Results from the modified akdalaite fit to the 6Fh PDF with 19 adjusted parameters

```
 * Mon Mar 25 10:00:51 2013

 ================================================================================
 PDF REFINEMENT
    Using PDFFIT version : 1.0-r6773-20111122
 ================================================================================
 --------------------------------------------------------------------------------
 PHASE 1 : UNNAMED
 --------------------------------------------------------------------------------
 Scale factor            : 1
    Particle diameter    : 35 A
    Step cutoff          : not applied
 Quad. corr. factor      : 0
 Lin. corr. factor       : 0
 Low r sigma ratio       : 0.461807 (0.1)
 R cutoff [A]            : 4.5
 Lattice parameters      : 5.95042 (0.0071)    5.95042 (0.0071)    9.1328 (0.02)
           & angles      : 90                  90                  120

 Atom positions & occupancies :
    FE    0.174916 (0.00091)  0.349832 (0.0018)   0.6365               1
    FE    0.650168 (0.0018)   0.825084 (0.00091)  0.6365               1
    FE    0.825084 (0.00091)  0.650168 (0.0018)   0.1365               1
    FE    0.349832 (0.0018)   0.174916 (0.00091)  0.1365               1
    FE    0.333333            0.666667            0.320721 (0.0029)    1.05785 (0.13)
    FE    0.666667            0.333333            0.820721 (0.0029)    1.05785 (0.13)
    FE    0.169787 (0.0033)   0.830213 (0.0033)   0.842818 (0.0023)    0.83144 (0.16)
    FE    0.830213 (0.0033)   0.169787 (0.0033)   0.342818 (0.0023)    0.83144 (0.16)
    O     0                   0                  -0.0344266 (0.0046)   1
    O     0                   0                   0.465573 (0.0046)    1
    O     0.333333            0.666667            0.779493 (0.0041)    1
    O     0.666667            0.333333            0.279493 (0.0041)    1
    O     0.167312 (0.0026)   0.832688 (0.0026)   0.233612 (0.0033)    1
    O     0.167312 (0.0026)   0.334623 (0.0051)   0.233612 (0.0033)    1
    O     0.665377 (0.0051)   0.832688 (0.0026)   0.233612 (0.0033)    1
    O     0.832688 (0.0026)   0.167312 (0.0026)   0.733612 (0.0033)    1
    O     0.832688 (0.0026)   0.665377 (0.0051)   0.733612 (0.0033)    1
    O     0.334623 (0.0051)   0.167312 (0.0026)   0.733612 (0.0033)    1
    O     0.528762 (0.0019)   0.471238 (0.0019)   0.971195 (0.0019)    1
    O     0.528762 (0.0019)   0.0575232 (0.0038)  0.971195 (0.0019)    1
    O     0.942477 (0.0038)   0.471238 (0.0019)   0.971195 (0.0019)    1
    O     0.471238 (0.0019)   0.528762 (0.0019)   0.471195 (0.0019)    1
    O     0.471238 (0.0019)   0.942477 (0.0038)   0.471195 (0.0019)    1
    O     0.0575232 (0.0038)  0.528762 (0.0019)   0.471195 (0.0019)    1

 Anisotropic temperature factors :
    FE    0.00697294 (0.00075) 0.00697294 (0.00075) 0.00697294 (0.00075)
    FE    0.00697294 (0.00075) 0.00697294 (0.00075) 0.00697294 (0.00075)
    FE    0.00697294 (0.00075) 0.00697294 (0.00075) 0.00697294 (0.00075)
    FE    0.00697294 (0.00075) 0.00697294 (0.00075) 0.00697294 (0.00075)
    FE    0.00697294 (0.00075) 0.00697294 (0.00075) 0.00697294 (0.00075)
    FE    0.00697294 (0.00075) 0.00697294 (0.00075) 0.00697294 (0.00075)
    FE    0.00697294 (0.00075) 0.00697294 (0.00075) 0.00697294 (0.00075)
    FE    0.00697294 (0.00075) 0.00697294 (0.00075) 0.00697294 (0.00075)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
    O     0.00563329 (0.0014) 0.00563329 (0.0014) 0.00563329 (0.0014)
```

```
------------------------------------------------------------------------
DATA SET : 1 (string)
------------------------------------------------------------------------
Data range in r [A]    : 1.38      -> 20              Step dr  : 0.02
Calculated range       : 1.38      -> 21.7952
Refinement r range     : 1.38      -> 20              Data pts : 0       -> 931
Reduced chi squared    : 0.270855
Rw - value             : 0.328578


Experimental settings  :
  Radiation            : X-Rays
  Termination at Qmax   : 21 A**-1
  DQ dampening Qdamp    : 0.0797513 (0.0059) A**-1
  DQ broadening Qbroad  : 0.069 A**-1
  Scale factor         : 1.46023 (0.071)

Selected phases and atoms for this data set :
  Phase 1 :
    Atoms (i) :   FE   O
    Atoms (j) :   FE   O

Relative phase content in terms of
          atoms                    unit cells              mass
Phase 1 : 1                        1                       1


------------------------------------------------------------------------
PARAMETER INFORMATION :
------------------------------------------------------------------------
Number of constraints        : 147
Number of refined parameters : 19
Number of fixed parameters   : 3

Refinement parameters :
  1: 1.46023 (0.071)         2: 0.0797513 (0.0059)      4: 5.95042 (0.0071)
  5: 9.1328 (0.02)           6: 0.461807 (0.1)          8: 35
 11: 0.174916 (0.00091)     12: 0.6365                 13: 0.320721 (0.0029)
 14: 0.169787 (0.0033)      15: 0.842818 (0.0023)      16: -0.0344266 (0.0046)
 17: 0.779493 (0.0041)      18: 0.167312 (0.0026)      19: 0.233612 (0.0033)
 20: 0.528762 (0.0019)      21: 0.971195 (0.0019)      100: 0.00697294 (0.00075)
200: 0.00563329 (0.0014)    301: 1                     302: 1.05785 (0.13)
303: 0.83144 (0.16)
------------------------------------------------------------------------
REFINEMENT INFORMATION:
------------------------------------------------------------------------
Number of iterations : 22
Reduced chi squared  : 0.268319
Rw - value           : 0.327036

Correlations greater than 0.8 :

   *** none ***
========================================================================
```