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Supporting information for article:

Background optimization of powder electron diffraction to implement e-PDF technique and study the local structure of iron oxide nanocrystals

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Figure S1 TEM bright field images of dispersed as-synthesized nanoparticles showing the spherical morphology.



Figure S2 Illumination of agglomerated as-synthesized nanoparticles using a parallel probe formed by 50 µm condenser aperture.

By studying the Electron Loss Near Edge Structure (ELNES) of L-ionization edges related to Fe, the formal oxidation state of the as-synthesized nanoparticles is determined. The electron transition from

spin-orbit split levels $(2P_{1/2} \text{ and } 2P_{3/2})$ to unoccupied 3d levels show characteristic L₃ and L₂ white line features that are sensitive to the local oxidation (Leapman *et al.*, 1980; Colliex *et al.*, 1991; Van Aken & Liebscher, 2002). Several methods have been adopted to relate the integrated intensity ratio of L_{2,3} edges to oxidation state (Riedl *et al.*, 2006). In the current study, second derivative method (Hosoi *et al.*, 1985; Botton *et al.*, 1995) was found to be a faster and more reliable approach. From the positive contributions of the area underneath L₃ and L₂ peaks, White Lines Ratio (WLR) was measured as 4.76 for the as-synthesized nanoparticles shown in Fig. S3a. To extract the nominal oxidation state of the nanoparticles, WLR was obtained from different standard reference iron oxide powder samples and compared as in Fig. S3b. The literature values (Colliex *et al.*, 1991) of WLR related to reference samples are slightly larger than shown in Fig. S3b and it could be due to adaptation of different model in isolating white lines peak intensities from the background.



Figure S3 Comparison of EELS White Lines Ratio (WLR) obtained from as-synthesized and standard reference iron oxide nanoparticles. (a) illustrates the positive contribution of Fe-L₃ and L₂ peaks after the second derivative of intensities acquired from one of the regions of interest (ROI) of as-synthesized nanoparticles. The WLR is performed from various ROIs' and represented by a circle filled with red (α -Fe₂O₃ std.), green (γ -Fe₂O₃ std.), grey (as-synthesized), and magenta (Fe₃O₄ std.)

shown in (b). The error bars are estimated from the variation of measured WLR between different regions.





Figure S4 Comparison of refined e-PDF G(r) profiles obtained at various regions of interest (ROI) using 300 kV and 80 kV electron beam energy. Related $\phi(q)$ profiles were overlaid in Fig. 6.





Figure S5 Comparison of refined e-PDF G(r) profiles obtained at various regions of interest (ROI) using 300 kV and 80 kV electron beam energy. Related $\phi(q)$ profiles were overlaid in Fig. 6.



Figure S6 Comparison of $G(r)_{diff}$ of 80 kV e-PDF profiles shown in Fig. S4 and S5. Majority of the difference is found in low-r region (up to 5 Å) between the refined G(r) profiles that have undergone single type-A and double type-B background subtraction. Beyond 5 Å interatomic distance range, the difference is not significant.



Figure S7 Final I(q) scattering intensity shown in Fig. 5(c) after undergoing type-A followed by type-B background subtraction and mean scattering factor, $N_0(f^2(q))$ fitted at the higher angle (about last one third of the q range).



Figure S8 Underneath carbon intensity profiles obtained at 300 kV and 80 kV.

Table S1Refined parameters of 300 kV e-PDF profiles generated for a damping range of 0 to 0.5in various Region of interest. Profile with lowest R_w is considered as optimum solution as plotted inFig. 4.

			Region	of interest	- 1 with do	amping = ()				
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U ₃₃	U _{iso}	S.O.F.		
Fe1	8b	0.7460	0.9983	0.1200	0.0063	0.0147	0.0037	0.008	0.702		
Fe2	4a	0.6297	0.6297		0.0034	0.0034	0.0007	0.002	0.497		
Fe3	8b	0.3703	0.8668	0.9870	0.0029	0.0043	0.0054	0.004	0.621		
Fe4	4a	0.1343	0.1343		0.0069	0.0069	0.0328	0.016	0.333		
01	8b	0.6273	0.8642	0.9786	0.0385	0.0189	0.0011	0.020	1		
02	8b	0.1205	0.3725	0.9987	0.0031	0.0096	0.0001	0.004	1		
03	8b	0.1279	0.8737	0.0074	0.0225	0.0321	0.0135	0.023	1		
O4	8b	0.3695	0.6323	0.9997	0.0217	0.0357	0.0140	0.024	1		
Region of interest - 1 with damping $= 0.1$											
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U_{33}	U _{iso}	S.O.F.		
Fe1	8b	0.7447	0.9998	0.1193	0.0069	0.0128	0.0083	0.009	0.720		
Fe2	4a	0.6263	0.6263		0.0085	0.0085	0.0010	0.006	0.579		
Fe3	8b	0.3679	0.8659	0.9859	0.0032	0.0071	0.0115	0.007	0.606		
Fe4	4a	0.1366	0.1366		0.0131	0.0131	0.0220	0.016	0.333		
01	8b	0.6208	0.8690	0.9784	0.0131	0.0197	0.0028	0.012	1		
02	8b	0.1175	0.3782	0.9973	0.0207	0.0288	0.0009	0.017	1		
03	8b	0.1289	0.8683	0.0139	0.0206	0.0230	0.0057	0.016	1		

$\mathbf{O}_{\mathbf{T}}$ 00 0.5001 0.0251 0.5905 0.0117 0.0105 0.0007 0.011	J4	0.014	0.008/	0.0189	0.014/	0.9965	0.6234	0.3664	86	04
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			Region of	f interest -	- 1 with da	mping = 0	.2		
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U_{33}	U_{iso}	S.O.F.
Fe1	8b	0.7450	1.0005	0.1183	0.0081	0.0148	0.0157	0.013	0.702
Fe2	4a	0.6289	0.6289		0.0074	0.0074	0.0056	0.007	0.540
Fe3	8b	0.3698	0.8654	0.9862	0.0134	0.0054	0.0084	0.009	0.562
Fe4	4a	0.1328	0.1328		0.0129	0.0129	0.0544	0.027	0.333
01	8b	0.6236	0.8679	0.9806	0.0373	0.0237	0.0052	0.022	1
02	8b	0.1140	0.3943	1.0020	0.0136	0.0210	0.0190	0.018	1
03	8b	0.1326	0.8698	0.0156	0.0083	0.0109	0.0092	0.009	1
O4	8b	0.3672	0.6223	0.9919	0.0222	0.0212	0.0079	0.017	1
			Region of	f interest -	l with da	mping = 0	.3		
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U_{33}	U _{iso}	S.O.F.
Fe1	8b	0.7445	1.0059	0.1190	0.0088	0.0139	0.0216	0.015	0.709
Fe2	4a	0.6299	0.6299		0.0147	0.0147	0.0073	0.012	0.467
Fe3	8b	0.3672	0.8655	0.9857	0.0144	0.0094	0.0123	0.012	0.602
Fe4	4a	0.1270	0.1270		0.0062	0.0062	0.0274	0.013	0.333
01	8b	0.6175	0.8700	0.9828	0.0241	0.0307	0.0048	0.020	1
02	8b	0.1257	0.3854	0.9960	0.0422	0.0257	0.0202	0.029	1
03	8b	0.1408	0.8721	0.0170	0.0171	0.0236	0.0127	0.018	1
O4	8b	0.3669	0.6187	0.9927	0.0185	0.0137	0.0068	0.013	1
			Region of	mping = 0	.4				
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U ₃₃	U_{iso}	S.O.F.
Fe1	8b	0.7444	1.0068	0.1171	0.0087	0.0142	0.0273	0.017	0.712
Fe2	4a	0.6290	0.6290		0.0166	0.0166	0.0124	0.015	0.463
Fe3	8b	0.3658	0.8673	0.9878	0.0145	0.0138	0.0153	0.015	0.600
Fe4	4a	0.1281	0.1281		0.0096	0.0096	0.0266	0.015	0.333
01	8b	0.6157	0.8722	0.9829	0.0158	0.0381	0.0068	0.020	1
02	8b	0.1285	0.3825	1.0001	0.0583	0.0291	0.0269	0.038	1
03	8b	0.1441	0.8749	0.0170	0.0115	0.0229	0.0143	0.016	1
04	8b	0.3654	0.6198	0.9945	0.0161	0.0179	0.0134	0.016	1
			Region of	f interest -	- 1 with da	mping = 0	.5		
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U ₃₃	U _{iso}	S.O.F.
Fe1	8b	0.7430	1.0066	0.1189	0.0102	0.0153	0.0331	0.020	0.712
Fe2	4a	0.6261	0.6261		0.0198	0.0198	0.0162	0.019	0.450
Fe3	8b	0.3638	0.8681	0.9912	0.0127	0.0188	0.0213	0.018	0.597
Fe4	4a	0.1287	0.1287		0.0109	0.0109	0.0276	0.016	0.333
01	8b	0.6116	0.8727	0.9830	0.0132	0.0368	0.0099	0.020	1
02	8b	0.1343	0.3776	1.0036	0.0488	0.0598	0.0241	0.044	1
03	8b	0.1440	0.8748	0.0181	0.0126	0.0271	0.0115	0.017	1
O4	8b	0.3644	0.6208	0.9964	0.0124	0.0179	0.0221	0.017	1

Damping =	0	0.1	0.2	0.3	0.4	0.5
scale factor	0.709	0.664	0.693	0.724	0.729	0.739
a (Å)	8.3456	8.3466	8.3446	8.3373	8.3493	8.3389
c (Å)	8.2930	8.2840	8.2858	8.3042	8.2996	8.3016
δ_2	3.42	3.31	3.12	2.44	2.51	2.73
$Q_{damp}(A^{-1})$	0.04524	0.03884	0.03921	0.04731	0.04703	0.04752
$Q_{broad}(\AA^{-1})$	0.00711	0.01187	0.00383	0.00123	0.00054	0.00072
R_w (%)	13.79	11.38	10.51	11.29	12.38	12.56

$$Q_{max}(\hat{A}^{-1}) = 19$$
; Range $(\hat{A}) = 1.2 - 50$; spdiameter $(\hat{A}) = 52.11$ (fixed);

		Region of interest - 2 with damping $= 0$										
Atom	Site	x	у	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.			
Fe1	8b	0.7470	0.9974	0.1208	0.0071	0.0096	0.0081	0.008	0.732			
Fe2	4a	0.6271	0.6271		0.0049	0.0049	0.0001	0.003	0.480			
Fe3	8b	0.3678	0.8687	0.9864	0.0059	0.0047	0.0052	0.005	0.661			
Fe4	4a	0.1278	0.1278		0.0064	0.0064	0.0227	0.012	0.333			
01	8b	0.6190	0.8636	0.9921	0.0318	0.0043	0.0024	0.013	1			
02	8b	0.1219	0.3729	0.9934	0.0109	0.0127	0.0065	0.010	1			
03	8b	0.1320	0.8733	0.0072	0.0171	0.0256	0.0152	0.019	1			
04	8b	0.3743	0.6339	0.9998	0.0194	0.0281	0.0185	0.022	1			
			Region of	f interest -	$\cdot 2$ with da	mping = 0	.1					
Atom	Site	x	у	z	U_{11}	U_{22}	U ₃₃	U _{iso}	S.O.F.			
Fe1	8b	0.7453	0.9965	0.1213	0.0085	0.0097	0.0092	0.009	0.730			
Fe2	4a	0.6271	0.6271		0.0094	0.0094	0.0061	0.008	0.470			
Fe3	8b	0.3684	0.8692	0.9803	0.0061	0.0070	0.0136	0.009	0.682			
Fe4	4a	0.1308	0.1308		0.0081	0.0081	0.0187	0.012	0.333			
01	8b	0.6123	0.8657	0.9837	0.0103	0.0066	0.0033	0.007	1			
02	8b	0.1158	0.3758	0.9921	0.0089	0.0188	0.0020	0.010	1			
03	8b	0.1296	0.8686	0.0043	0.0143	0.0177	0.0048	0.012	1			
04	8b	0.3697	0.6341	1.0030	0.0131	0.0173	0.0098	0.013	1			
			Region of	f interest -	$\cdot 2$ with da	mping = 0	.2					
Atom	Site	x	у	z	U_{11}	U_{22}	U ₃₃	U _{iso}	S.O.F.			
Fe1	8b	0.7504	0.9918	0.1166	0.0127	0.0145	0.0197	0.016	0.645			
Fe2	4a	0.6287	0.6287		0.0258	0.0258	0.0151	0.022	0.660			
Fe3	8b	0.3739	0.8660	0.9900	0.0077	0.0061	0.0039	0.006	0.306			
Fe4	4a	0.1334	0.1334		0.0048	0.0048	0.0286	0.013	0.333			
01	8b	0.6139	0.8590	0.9975	0.0665	0.0160	0.0183	0.034	1			
02	8b	0.1126	0.3711	1.0051	0.0188	0.0126	0.0179	0.016	1			
03	8b	0.1271	0.8756	0.0108	0.0327	0.0129	0.0238	0.023	1			
04	8b	0.3960	0.6473	1.0114	0.0188	0.0107	0.0117	0.014	1			
			Region of	of interest -	$\cdot 2$ with da	mping = 0	.3					
Atom	Site	x	У	z	<i>U</i> ₁₁	U_{22}	U_{33}	U_{iso}	S.O.F.			
Fe1	8b	0.7397	1.0019	0.1296	0.0136	0.0085	0.0136	0.012	0.652			
Fe2	4a	0.6168	0.6168		0.0047	0.0047	0.0091	0.006	0.302			
Fe3	8b	0.3759	0.8714	0.9923	0.0111	0.0207	0.0110	0.014	0.549			
Fe4	4a	0.1235	0.1235		0.0059	0.0059	0.0200	0.011	0.333			
01	8b	0.6044	0.8745	0.9807	0.0237	0.0077	0.0203	0.017	1			
02	8b	0.1063	0.3978	0.9900	0.0085	0.0141	0.0096	0.011	1			
03	8b	0.1166	0.8725	0.0007	0.0003	0.0232	0.0144	0.013	1			
04	8b	0.3746	0.6276	0.9789	0.0257	0.0179	0.0082	0.017	1			
			Region of	of interest -	$\cdot 2$ with da	mping = 0	.4					
Atom	Site	x	У	z	<i>U</i> ₁₁	U_{22}	U_{33}	U_{iso}	S.O.F.			
Fe1	8b	0.7541	0.9950	0.1152	0.0094	0.0237	0.0254	0.020	0.659			
Fe2	4a	0.6326	0.6326		0.0153	0.0153	0.0179	0.016	0.628			
Fe3	8b	0.3732	0.8663	0.9877	0.0114	0.0084	0.0074	0.009	0.341			
Fe4	4a	0.1325	0.1325		0.0070	0.0070	0.0433	0.019	0.333			
01	8b	0.6434	0.8708	0.9919	0.0091	0.0397	0.0087	0.019	1			
02	8b	0.1192	0.3778	1.0029	0.0090	0.0202	0.0290	0.019	1			
03	8b	0.1234	0.8792	0.0214	0.0356	0.0472	0.0038	0.029	1			
04	8b	0.3881	0.6318	0.9740	0.0562	0.0112	0.0203	0.029	1			

			Region o	f interest -	2 with dat	mping = 0	.5		
Atom	Site	x	У	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.
Fe1	8b	0.7456	1.0096	0.1199	0.0114	0.0241	0.0362	0.024	0.667
Fe2	4a	0.6315	0.6315		0.0108	0.0108	0.0051	0.009	0.273
Fe3	8b	0.3693	0.8662	0.9859	0.0192	0.0102	0.0190	0.016	0.527
Fe4	4a	0.1255	0.1255		0.0119	0.0119	0.0245	0.016	0.333
01	8b	0.6185	0.8641	0.9736	0.0089	0.0234	0.0197	0.017	1
02	8b	0.1257	0.3910	0.9949	0.0658	0.0219	0.0555	0.048	1
03	8b	0.1452	0.8702	0.0098	0.0198	0.0397	0.0310	0.030	1
04	8b	0.3728	0.6207	1.0009	0.0088	0.0445	0.0147	0.023	1

Damping =	0	0.1	0.2	0.3	0.4	0.5
scale factor	0.674	0.650	0.784	0.757	0.759	0.761
a (Å)	8.3506	8.3571	8.3397	8.3492	8.3540	8.3549
c (Å)	8.2947	8.2791	8.3207	8.2997	8.2885	8.2846
δ_2	3.47471	3.3586	1.80461	2.87121	2.4866	2.28811
$Q_{damp}(A^{-1})$	0.04196	0.03945	0.04467	0.04240	0.04160	0.04304
$Q_{broad}(A^{-1})$	0.02280	0.02156	0.01086	0.00106	0.00047	0.00081
$R_{w}(\%)$	16.45	13.52	12.99	12.01	11.35	11.95
0 (1)	$\frac{1}{1} = 10 \cdot \mathbf{R}^{-1}$	$(n^{2}) = 1$	2 50. and	and at an ()	-52.11(fine	.d).

 $Q_{max}(A^{-1}) = 19$; Range (A) = 1.2 - 50; spdiameter (A) = 52.11 (fixed);

	Region of interest - 3 with damping $= 0$										
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U ₃₃	U _{iso}	S.O.F.		
Fe1	8b	0.7464	0.9956	0.1206	0.0100	0.0106	0.0104	0.010	0.825		
Fe2	4a	0.6280	0.6280		0.0078	0.0078	0.0045	0.007	0.594		
Fe3	8b	0.3677	0.8694	0.9877	0.0085	0.0098	0.0097	0.009	0.709		
Fe4	4a	0.1285	0.1285		0.0101	0.0101	0.0151	0.012	0.333		
01	8b	0.6183	0.8616	0.9942	0.0229	0.0188	0.0224	0.021	1		
02	8b	0.1242	0.3724	0.9933	0.0089	0.0083	0.0103	0.009	1		
03	8b	0.1328	0.8709	0.0083	0.0121	0.0176	0.0139	0.015	1		
04	8b	0.3739	0.6337	0.9999	0.0114	0.0135	0.0135	0.013	1		
	Region of interest -3 with damping = 0.1										
Atom	Site	x	У	z	U_{11}	U_{22}	U_{33}	U _{iso}	S.O.F.		
Fe1	8b	0.7449	0.9959	0.1212	0.0087	0.0137	0.0091	0.010	0.705		
Fe2	4a	0.6296	0.6296		0.0094	0.0094	0.0004	0.006	0.655		
Fe3	8b	0.3677	0.8672	0.9845	0.0042	0.0075	0.0053	0.006	0.507		
Fe4	4a	0.1325	0.1325		0.0108	0.0108	0.0248	0.015	0.333		
01	8b	0.6232	0.8748	0.9858	0.0325	0.0282	0.0144	0.025	1		
02	8b	0.1082	0.3649	1.0027	0.0121	0.0216	0.0140	0.016	1		
03	8b	0.1317	0.8784	0.0050	0.0133	0.0260	0.0071	0.015	1		
04	8b	0.3710	0.6312	1.0035	0.0126	0.0146	0.0182	0.015	1		

			Region of	f interest -	3 with dan	nping = 0.	2		
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U ₃₃	U_{iso}	S.O.F.
Fe1	8b	0.7408	0.9979	0.1211	0.0192	0.0154	0.0053	0.013	0.663
Fe2	4a	0.6364	0.6364		0.0077	0.0077	0.0034	0.006	0.413
Fe3	8b	0.3697	0.8644	0.9864	0.0074	0.0093	0.0124	0.010	0.525
Fe4	4a	0.1203	0.1203		0.0067	0.0067	0.0095	0.008	0.333
01	8b	0.6139	0.8750	0.9806	0.0277	0.0313	0.0041	0.021	1
02	8b	0.1131	0.3804	0.9746	0.0625	0.0031	0.0423	0.036	1
03	8b	0.1313	0.8636	0.0043	0.0279	0.0268	0.0122	0.022	1
04	8b	0.3696	0.6236	0.9915	0.0104	0.0084	0.0021	0.007	1
			Region of	f interest -	3 with dan	nping = 0	3		
Atom	Site	x	У	z	<i>U</i> ₁₁	U_{22}	U ₃₃	U _{iso}	S.O.F.
Fe1	8b	0.7410	1.0019	0.1312	0.0163	0.0122	0.0222	0.017	0.643
Fe2	4a	0.6200	0.6200		0.0019	0.0019	0.0044	0.003	0.174
Fe3	8b	0.3791	0.8735	0.9914	0.0105	0.0201	0.0143	0.015	0.524
Fe4	4a	0.1117	0.1117		0.0050	0.0050	0.0119	0.007	0.333
01	8b	0.6216	0.8755	0.9921	0.0112	0.0301	0.0081	0.016	1
02	8b	0.1162	0.3641	0.9642	0.0269	0.0572	0.0894	0.058	1
03	8b	0.1166	0.8723	0.0105	0.0107	0.0284	0.0120	0.017	1
04	8b	0.3595	0.6321	0.9771	0.0129	0.0235	0.0061	0.014	1
			Region of	f interest -	3 with dan	nping = 0.4	4		
Atom	Site	x	у	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U_{iso}	S.O.F.
Fe1	8b	0.7425	1.0055	0.1301	0.0107	0.0224	0.0286	0.021	0.678
Fe2	4a	0.6351	0.6351		0.0038	0.0038	0.0027	0.003	0.241
Fe3	8b	0.3680	0.8672	0.9884	0.0142	0.0118	0.0147	0.014	0.544
Fe4	4a	0.1227	0.1227		0.0084	0.0084	0.0252	0.014	0.333
01	8b	0.6218	0.8652	0.9888	0.0220	0.0383	0.0202	0.027	1
02	8b	0.1230	0.3872	0.9901	0.0489	0.0231	0.0674	0.046	1
03	8b	0.1420	0.8805	0.0057	0.0159	0.0683	0.0259	0.037	1
04	8b	0.3724	0.6234	0.9899	0.0140	0.0251	0.0116	0.017	1
			Region	of interest	- 3 with da	imping = ().5		
Atom	Site	x	У	z	<i>U</i> ₁₁	U_{22}	U_{33}	U _{iso}	S.O.F.
Fe1	8b	0.7365	0.9996	0.1288	0.0269	0.0102	0.0267	0.021	0.626
Fe2	4a	0.6265	0.6265		0.0041	0.0041	0.0088	0.006	0.232
Fe3	8b	0.3775	0.8714	0.9895	0.0192	0.0267	0.0144	0.020	0.536
Fe4	4a	0.1142	0.1142		0.0087	0.0087	0.0194	0.012	0.333
01	8b	0.6273	0.8770	0.9918	0.0209	0.0217	0.0190	0.021	1
02	8b	0.1156	0.3634	0.9676	0.0517	0.0445	0.0913	0.062	1
03	8b	0.1204	0.8743	0.0070	0.0214	0.0402	0.0143	0.025	1
04	8b	0.3578	0.6366	0.9768	0.0104	0.0244	0.0102	0.015	1

Damping =	0	0.1	0.2	0.3	0.4	0.5
scale factor	0.638	0.652	0.698	0.749	0.720	0.739
a (Å)	8.3499	8.3423	8.3494	8.34041	8.3414	8.3430
c (Å)	8.2932	8.2917	8.2929	8.30052	8.2982	8.2959
δ_2	3.49	3.31	3.06	2.88	2.76	2.70
$Q_{damp}(A^{-1})$	0.05028	0.04856	0.04796	0.04779	0.04994	0.04983
$Q_{broad}(\AA^{-1})$	0.00206	0.00998	0.00175	0.00121	0.00124	0.00336

$$\frac{R_{w}(\%)}{Q_{max}(\AA^{-1})} = 19; Range(\AA) = 1.2 - 50; spdiameter(\AA) = 52.11(fixed);$$

	Region of interest - 4 with damping $= 0$											
Atom	Site	x	y	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.			
Fe1	8b	0.7474	0.9966	0.1214	0.0298	0.0122	0.0184	0.020	0.813			
Fe2	4a	0.6240	0.6240		0.0033	0.0033	0.0074	0.005	0.739			
Fe3	8b	0.3671	0.8723	0.9835	0.0016	0.0098	0.0053	0.006	0.609			
Fe4	4a	0.1299	0.1299		0.0037	0.0037	0.0068	0.005	0.333			
01	8b	0.6150	0.8675	0.9844	0.0475	0.0033	0.0023	0.018	1			
02	8b	0.1232	0.3756	0.9885	0.0309	0.0223	0.0033	0.019	1			
03	8b	0.1274	0.8754	0.0048	0.0111	0.0183	0.0152	0.015	1			
O4	8b	0.3706	0.6336	1.0004	0.0052	0.0215	0.0079	0.012	1			
			Region of	f interest -	4 with dan	nping = 0.	1					
Atom	Site	x	У	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.			
Fe1	8b	0.7463	0.9955	0.1180	0.0102	0.0075	0.0134	0.010	0.820			
Fe2	4a	0.6256	0.6256		0.0093	0.0093	0.0099	0.009	0.823			
Fe3	8b	0.3655	0.8714	0.9798	0.0049	0.0163	0.0156	0.012	0.786			
Fe4	4a	0.1307	0.1307		0.0045	0.0045	0.0218	0.010	0.333			
01	8b	0.6120	0.8682	0.9845	0.0015	0.0490	0.0040	0.018	1			
02	8b	0.1179	0.3799	0.9905	0.0168	0.0306	0.0139	0.020	1			
03	8b	0.1318	0.8777	0.0061	0.0410	0.0111	0.0077	0.020	1			
04	8b	0.3727	0.6313	1.0064	0.0018	0.0085	0.0041	0.005	1			
			Region	of interest	- 4 with da	imping = (0.2					
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U_{33}	U _{iso}	S.O.F.			
Fe1	8b	0.7372	0.9999	0.1207	0.0175	0.0113	0.0088	0.013	0.687			
Fe2	4a	0.6334	0.6334		0.0048	0.0048	0.0019	0.004	0.409			
Fe3	8b	0.3622	0.8739	0.9843	0.0157	0.0112	0.0154	0.014	0.696			
Fe4	4a	0.1278	0.1278		0.0075	0.0075	0.0069	0.007	0.333			
01	8b	0.6165	0.8695	0.9799	0.0125	0.0412	0.0045	0.019	1			
02	8b	0.0979	0.3993	1.0036	0.0219	0.0238	0.0030	0.016	1			
03	8b	0.1486	0.8715	0.0119	0.0346	0.0093	0.0065	0.017	1			
04	8b	0.3821	0.6141	0.9944	0.0060	0.0055	0.0045	0.005	1			
			Region	of interest	- 4 with da	imping = ().3					
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U_{33}	U _{iso}	S.O.F.			
Fe1	8b	0.7422	0.9959	0.1082	0.0063	0.0097	0.0358	0.017	0.717			
Fe2	4a	0.6340	0.6340		0.0135	0.0135	0.0122	0.013	0.680			
Fe3	8b	0.3677	0.8714	0.9796	0.0060	0.0111	0.0089	0.009	0.468			
Fe4	4a	0.1228	0.1228		0.0082	0.0082	0.0083	0.008	0.333			
01	8b	0.6164	0.8778	0.9788	0.0122	0.0315	0.0133	0.019	1			
02	8b	0.1205	0.3850	0.9827	0.0376	0.0174	0.0230	0.026	1			
03	8b	0.1124	0.8821	0.0161	0.0322	0.0086	0.0121	0.018	1			
O4	8b	0.3773	0.6377	0.9979	0.0151	0.0083	0.0128	0.012	1			
			Region	of interest	- 4 with da	imping = ().4					
Atom	Site	x	У	z	<i>U</i> ₁₁	U_{22}	U_{33}	U _{iso}	S.O.F .			
Fe1	8b	0.7326	1.0034	0.1202	0.0330	0.0087	0.0152	0.019	0.679			
Fe2	4a	0.6389	0.6389		0.0119	0.0119	0.0143	0.013	0.414			
Fe3	8b	0.3649	0.8729	0.9869	0.0213	0.0139	0.0119	0.016	0.505			
Fe4	4a	0.1228	0.1228		0.0054	0.0054	0.0124	0.008	0.333			
01	8b	0.6308	0.8702	0.9646	0.0756	0.0091	0.0180	0.034	1			
02	8b	0.1167	0.3852	0.9998	0.0093	0.0109	0.0144	0.012	1			
03	8b	0.1531	0.8687	0.0255	0.0704	0.0126	0.0079	0.030	1			
~ .	01-	0 2 2 0 2	0.6114	0 9947	0.0103	0.0110	0.0154	0.012	1			

			Region o	f interest -	4 with dat	mping = 0	.5		
Atom	Site	x	У	ζ	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.
Fe1	8b	0.7460	1.0013	0.1130	0.0258	0.0101	0.0475	0.028	0.660
Fe2	4a	0.6348	0.6348		0.0207	0.0207	0.0245	0.022	0.640
Fe3	8b	0.3628	0.8757	0.9880	0.0142	0.0152	0.0108	0.013	0.337
Fe4	4a	0.1226	0.1226		0.0102	0.0102	0.0140	0.011	0.333
01	8b	0.6381	0.8799	0.9676	0.0438	0.0194	0.0117	0.025	1
02	8b	0.1233	0.3793	1.0014	0.0208	0.0168	0.0182	0.019	1
03	8b	0.1673	0.8731	0.0282	0.1094	0.0150	0.0144	0.046	1
04	8b	0.3893	0.6145	0.9909	0.0064	0.0287	0.0234	0.019	1

Damping =	0	0.1	0.2	0.3	0.4	0.5
scale factor	0.774	0.673	0.799	0.772	0.845	0.880
a (Å)	8.3438	8.3473	8.3449	8.34593	8.3480	8.3457
c (Å)	8.2962	8.2934	8.2959	8.30082	8.2979	8.3037
δ_2	2.86	3.32	3.11	3.08	2.95	2.84
$Q_{damp}(A^{-1})$	0.04911	0.04556	0.04539	0.04214	0.04394	0.04506
$Q_{broad}(\AA^{-1})$	0.00273	0.00281	0.00643	0.01909	0.00118	0.00125
$R_{w}(\%)$	29.33	17.48	14.80	14.09	11.70	13.16
0 (1)	$\frac{1}{1} - 10 \cdot \mathbf{P}_{ab}$	$a_{\alpha}(\mathbf{A}) = 1^{\prime}$	$2 50 \cdot cndi$	amatar (Å)	-52.11(fixe	d).

			Region	of interest	- 5 with de	amping = 0	0		
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U_{33}	U _{iso}	S.O.F.
Fe1	8b	0.7478	0.9971	0.1221	0.0096	0.0109	0.0079	0.009	0.915
Fe2	4a	0.6234	0.6234		0.0103	0.0103	0.0100	0.010	0.795
Fe3	8b	0.3675	0.8708	0.9872	0.0077	0.0098	0.0041	0.007	0.861
Fe4	4a	0.1292	0.1292		0.0164	0.0164	0.0115	0.015	0.333
01	8b	0.6183	0.8652	0.9938	0.0218	0.0021	0.0018	0.009	1
02	8b	0.1224	0.3729	0.9919	0.0141	0.0112	0.0021	0.009	1
03	8b	0.1301	0.8732	0.0061	0.0105	0.0205	0.0046	0.012	1
04	8b	0.3749	0.6329	0.9996	0.0144	0.0143	0.0025	0.010	1
			Region of	f interest ·	- 5 with da	mping = 0	.1		
Atom	Site	x	У	z	<i>U</i> ₁₁	U_{22}	U_{33}	U_{iso}	S.O.F.
Fe1	8b	0.7465	0.9959	0.1210	0.0088	0.0143	0.0094	0.011	0.773
Fe2	4a	0.6235	0.6235		0.0055	0.0055	0.0012	0.004	0.511
Fe3	8b	0.3657	0.8685	0.9830	0.0070	0.0117	0.0119	0.010	0.718
Fe4	4a	0.1323	0.1323		0.0122	0.0122	0.0056	0.010	0.333
01	8b	0.6144	0.8655	0.9920	0.0057	0.0137	0.0243	0.015	1
02	8b	0.1179	0.3749	0.9885	0.0172	0.0179	0.0083	0.014	1
03	8b	0.1285	0.8702	0.0061	0.0158	0.0184	0.0052	0.013	1
04	8b	0.3744	0.6323	1.0017	0.0107	0.0306	0.0108	0.017	1
			Region of	f interest	- 5 with da	mping = 0	.2		
Atom	Site	x	У	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F .
Fe1	8b	0.7417	0.9950	0.1223	0.0099	0.0209	0.0054	0.012	0.696
Fe2	4a	0.6257	0.6257		0.0120	0.0120	0.0060	0.010	0.488

Fe3	8b	0.3678	0.8692	0.9809	0.0084	0.0098	0.0178	0.012	0.641
Fe4	4a	0.1352	0.1352		0.0077	0.0077	0.0045	0.007	0.333
01	8b	0.6054	0.8695	0.9952	0.0229	0.0054	0.0184	0.016	1
02	8b	0.1101	0.3919	0.9852	0.0246	0.0152	0.0129	0.018	1
03	8b	0.1350	0.8765	0.0068	0.0172	0.0220	0.0073	0.016	1
04	8b	0.3655	0.6242	0.9989	0.0124	0.0080	0.0088	0.010	1
			Region of	f interest -	5 with dat	mping = 0	.3		
Atom	Site	x	У	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.
Fe1	8b	0.7441	0.9928	0.1161	0.0090	0.0218	0.0124	0.014	0.703
Fe2	4a	0.6309	0.6309		0.0122	0.0122	0.0365	0.020	0.607
Fe3	8b	0.3656	0.8726	0.9900	0.0035	0.0101	0.0170	0.010	0.477
Fe4	4a	0.1375	0.1375		0.0215	0.0215	0.0190	0.021	0.333
01	8b	0.6262	0.8673	0.9833	0.0259	0.0145	0.0346	0.025	1
02	8b	0.0997	0.3844	0.9832	0.0051	0.0150	0.0133	0.011	1
03	8b	0.1179	0.8621	0.0040	0.0185	0.0221	0.0045	0.015	1
O4	8b	0.3701	0.6330	0.9916	0.0079	0.0139	0.0213	0.014	1
			Region of	f interest -	5 with dat	mping = 0.	.4		
Atom	Site	x	У	z	<i>U</i> ₁₁	U_{22}	U_{33}	U _{iso}	S.O.F.
Fe1	8b	0.7383	1.0031	0.1235	0.0310	0.0115	0.0107	0.018	0.719
Fe2	4a	0.6296	0.6296		0.0221	0.0221	0.0067	0.017	0.573
Fe3	8b	0.3666	0.8701	0.9843	0.0257	0.0223	0.0123	0.020	0.602
Fe4	4a	0.1238	0.1238		0.0116	0.0116	0.0211	0.015	0.333
01	8b	0.6200	0.8694	0.9829	0.0120	0.0262	0.0120	0.017	1
02	8b	0.1291	0.3906	0.9875	0.0519	0.0024	0.0224	0.026	1
03	8b	0.1413	0.8751	0.0161	0.0235	0.0090	0.0211	0.018	1
04	8b	0.3716	0.6219	0.9935	0.0142	0.0321	0.0060	0.017	1
			Region of	f interest -	\cdot 5 with dat	mping = 0.	.5		
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U_{33}	U_{iso}	S.O.F.
Fe1	8b	0.7387	0.9951	0.1214	0.0386	0.0063	0.0189	0.021	0.741
Fe2	4a	0.6402	0.6402		0.0237	0.0237	0.0380	0.028	0.486
Fe3	8b	0.3699	0.8698	0.9852	0.0130	0.0269	0.0151	0.018	0.582
Fe4	4a	0.1220	0.1220		0.0087	0.0087	0.0298	0.016	0.333
01	8b	0.6300	0.8661	0.9913	0.0167	0.0483	0.0397	0.035	1
02	8b	0.1172	0.3831	0.9978	0.0131	0.0137	0.0173	0.015	1
03	8b	0.1369	0.8662	0.0243	0.0203	0.0199	0.0061	0.015	1
04	8b	0.3804	0.6268	0.9909	0.0125	0.0189	0.0155	0.016	1

Damping =	0	0.1	0.2	0.3	0.4	0.5
scale factor	0.592	0.661	0.704	0.726	0.711	0.712
a (Å)	8.3470	8.3403	8.3467	8.34329	8.3458	8.3464
c (Å)	8.2972	8.2910	8.2952	8.29859	8.2903	8.2945
δ_2	3.43	3.21	3.18	3.04	2.94	2.95
$Q_{damp}(A^{-1})$	0.04657	0.04565	0.04565	0.04771	0.05026	0.05014
$Q_{broad}(\AA^{-1})$	0.01337	0.00786	0.01036	0.00426	0.00124	0.00124
$R_w(\%)$	23.23	15.14	13.23	11.71	11.96	12.78
$Q_{max}(A)$	⁻¹) = 19; Ran	ige (Å) = 1.1	2 – 50 ; spdi	ameter (Å)	= 52.11(fixe	ed);

Region of interest - 6 with damping = 0										
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U ₃₃	U _{iso}	S.O.F.	
Fe1	8b	0.7473	0.9977	0.1208	0.0070	0.0081	0.0145	0.010	0.890	
Fe2	4a	0.6265	0.6265		0.0029	0.0029	0.0096	0.005	0.820	

Fe3	8b	0.3651	0.8727	0.9839	0.0074	0.0133	0.0109	0.011	0.844
Fe4	4a	0.1248	0.1248		0.0035	0.0035	0.0920	0.033	0.333
01	8b	0.6187	0.8624	0.9887	0.0197	0.0025	0.0042	0.009	1
02	8b	0.1196	0.3711	0.9946	0.0061	0.0132	0.0067	0.009	1
03	8b	0.1341	0.8764	0.0014	0.0163	0.0201	0.0120	0.016	1
O4	8b	0.3727	0.6413	1.0024	0.0050	0.0049	0.0062	0.005	1
			Region of	f interest -	6 with dan	nping = 0.	1		
Atom	Site	x	у	z	<i>U</i> ₁₁	U ₂₂	U_{33}	U _{iso}	S.O.F.
Fe1	8b	0.7455	0.9967	0.1183	0.0064	0.0088	0.0228	0.013	0.819
Fe2	4a	0.6269	0.6269		0.0072	0.0072	0.0109	0.008	0.734
Fe3	8b	0.3646	0.8724	0.9807	0.0029	0.0171	0.0230	0.014	0.803
Fe4	4a	0.1326	0.1326		0.0101	0.0101	0.0074	0.009	0.333
01	8b	0.6125	0.8672	0.9879	0.0069	0.0073	0.0114	0.009	1
02	8b	0.1139	0.3811	0.9929	0.0116	0.0224	0.0073	0.014	1
03	8b 01-	0.1367	0.8780	0.0062	0.0269	0.0169	0.0112	0.018	1
04	80	0.3/26	0.6323	1.0051	0.0063	0.0184	0.0104	0.012	I
	G •4		Region	oj interest	- 0 wiin aa	imping = 0	<i>1.2</i>		COE
Atom E 1	Site	x	<u>y</u>	Z	$\frac{U_{11}}{0.0065}$	U_{22}	$\frac{U_{33}}{0.0258}$	$\frac{U_{iso}}{0.014}$	S.U.F.
rei Fol	80 40	0.7417	0.9980	0.1127	0.0005	0.0085	0.0258	0.014	0.699
ге2 Бо3	4a 8h	0.0529	0.0529	0.0705	0.0108	0.0108	0.0002	0.009	0.005
res Fol	00 /a	0.3062	0.8723	0.9795	0.0100	0.0127	0.0144	0.012	0.338
01	4a 8h	0.1202	0.1202	0 9755	0.0052	0.0032	0.0122	0.000	0.335
01	8b	0.0224	0.3969	1 0003	0.0105	0.0437	0.0035	0.022	1
03	8b	0.1412	0.8842	0.0177	0.0524	0.0019	0.0072	0.020	1
04	8b	0.3722	0.6313	1.0001	0.0104	0.0050	0.0085	0.008	1
			Region	of interest	- 6 with da	mping = ().3		
Atom	Site	x	у	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.
Fe1	8b	0.7461	0.9986	0.1118	0.0108	0.0107	0.0341	0.019	0.686
Fe2	4a	0.6354	0.6354		0.0156	0.0156	0.0178	0.016	0.720
Fe3	8b	0.3685	0.8697	0.9878	0.0104	0.0114	0.0040	0.009	0.301
Fe4	4a	0.1237	0.1237		0.0103	0.0103	0.0115	0.011	0.333
01	8b	0.6420	0.8821	0.9719	0.0222	0.0278	0.0043	0.018	1
02	8b	0.1217	0.3777	0.9979	0.0217	0.0161	0.0166	0.018	l
03	8b 01-	0.1483	0.8743	0.0251	0.0211	0.0215	0.0092	0.017	1
04	80	0.3817	0.02/4	0.9931	0.0135	0.01/4	0.0102	0.010	1
	G •4		Region	oj interest	- 0 wiin aa	imping = 0	<i>1.4</i>		COE
Atom	Site	x	<u>y</u>	Z	U_{11}	U_{22}	U_{33}		S.O.F.
rel E-2	80 40	0.7458	0.9984	0.1112	0.0164	0.0103	0.0383	0.022	0.633
rez Fo2	4a 82	0.0301	0.0301	0 0802	0.0103	0.0103	0.0220	0.018	0.015
Fed	00 49	0.3070	0.0713 0 1774	0.2072	0.0120	0.0108	0.0002	0.012	0.320
01	ча 8h	0.6418	0.8816	0.9723	0.0210	0.0307	0.0046	0.019	1
0^{1}	8b	0.1206	0.3777	0.9991	0.0231	0.0147	0.0156	0.018	1
03	8b	0.1513	0.8750	0.0276	0.0150	0.0211	0.0103	0.015	1
04	8b	0.3838	0.6229	0.9919	0.0116	0.0290	0.0170	0.019	1
			Region	of interest	- 6 with da	mping = ().5		
Atom	Site	x	у	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	Uiso	S.O.F.
Fe1	8b	0.7445	1.0012	0.1112	0.0181	0.0134	0.0435	0.025	0.651
Fe2	4a	0.6365	0.6365		0.0144	0.0144	0.0230	0.017	0.597
Fe3	8b	0.3668	0.8720	0.9880	0.0164	0.0169	0.0079	0.014	0.309
Fe4	4a	0.1239	0.1239		0.0161	0.0161	0.0122	0.015	0.333
01	8b	0.6412	0.8827	0.9727	0.0376	0.0313	0.0043	0.024	1
02	8b	0.1209	0.3793	0.9986	0.0226	0.0184	0.0156	0.019	1
03	8b	0.1524	0.8757	0.0282	0.0194	0.0132	0.0155	0.016	1
04	8b	0.3825	0.6239	0.9925	0.0199	0.0314	0.0229	0.025	1

Damping =	0	0.1	0.2	0.3	0.4	0.5				
scale factor	0.619	0.647	0.748	0.794	0.815	0.805				
a (Å)	8.3429	8.3475	8.3453	8.34511	8.3455	8.3480				
c (Å)	8.2987	8.2950	8.2924	8.29875	8.2935	8.2978				
δ_2	3.49	3.38	3.21	2.83	2.68	2.80				
$Q_{damp}(A^{-1})$	0.04493	0.04641	0.04654	0.04642	0.04827	0.04655				
$Q_{broad}(\AA^{-1})$	0.01500	0.00024	0.00271	0.00290	0.00221	0.00196				
$R_{w}(\%)$	20.61	16.99	14.10	13.05	13.63	13.70				
$Q_{max}(\hat{A}^{-1}) = 19$; Range $(\hat{A}) = 1.2 - 50$; spdiameter $(\hat{A}) = 52.11$ (fixed);										

Table S2Refined parameters related to the profiles shown in Fig. S4 and S5

				300 k)	$V(\overline{ROI-1})$							
	$Q_{max}(\dot{A}^{-1}) = 19$; Range (\dot{A}) = 1.2 – 50; scale factor = 0.693; a (\dot{A}) = 8.3446;											
$c(\mathbf{A}) = 8.2858; \ damping = 0.2; \ \delta_2 = 3.12; \ \mathbf{O}, \ (\mathbf{A}^{-1}) = 0.03921; \ \mathbf{O}, \ (\mathbf{A}^{-1}) = 0.00383;$												
spliameter $(Å) = 52.11$ (fixed); $R_w(\%) = 10.51$												
Atom Site x v z U_{11} U_{22} U_{22} U_{23} S.O.F.												
Fo1	8h	A 0.7450	<u> </u>	<u> </u>	0.0081	0.0148	0.0157	0.012	0.702			
Fel Fo2	00 /a	0.7430	0.6280	0.1165	0.0081	0.0148	0.0157	0.013	0.702			
Fc2 Fo3	7a 8h	0.0289	0.0289	0.0862	0.0074 0.0134	0.0074	0.0050	0.007	0.540			
гез Бол	40	0.3098	0.0004	0.9802	0.0134	0.0034	0.0084	0.009	0.302			
D1	4a 8h	0.1326	0.1328	0.0806	0.0129	0.0129	0.0344	0.027	0.555			
	80 85	0.0230	0.8079	1.0020	0.0373	0.0237	0.0032	0.022	1			
02	80 81	0.1140	0.3943	0.0156	0.0130	0.0210	0.0190	0.018	1			
03	80 8h	0.1320	0.8098	0.0130	0.0085	0.0109	0.0092	0.009	1			
04	80	0.3072	4V (DOL 1	$\frac{0.9919}{0.9919}$	0.0222	0.0212	0.0079	0.017	1			
		001	κν (KOI-1) ajter type	e-A backgr	ouna subii	raction					
	Q_{max}	4 ⁻¹) = 19;	Range (Å) = 1.2 - 5	0; scale f a	actor = 0.5	77; a (Å)	= 8.3567	;			
c (Å)	= 8.279	95; dampi	ng = 0.4; d	$S_2 = 3.05$:	$O_{1} (A^{-1})$	= 0.0512	4: 0 , ,(4	$\mathbf{\mathring{4}}^{-1}$) = 0.	00242;			
		si si	odiameter	(A) = 52.1	∼aamp (1 (fixed): 1	, R w(%) = 2	20.47	,	,			
Atom	Site	r	v	7	U	Uaa	Uaa	Uine	S.O.F.			
Fol	01	~~	J	40	νn	022	033	<i>c iso</i>	0.622			
	- AN	0 7401	0 9973	0 1159	0.0091	0.0176	0 0299	0.019	0.633			
Fel Fel	80 4a	0.7401 0.6369	0.9973 0.6369	0.1159	0.0091	$0.0176 \\ 0.0037$	0.0299	0.019	0.633			
Fe2 Fe3	80 4a 8b	0.7401 0.6369 0.3713	0.9973 0.6369 0.8685	0.1159	0.0091 0.0037 0.0206	0.0176 0.0037 0.0124	0.0299 0.0000 0.0191	0.019 0.002 0.017	0.633 0.222 0.523			
Fe2 Fe3 Fe4	80 4a 8b 4a	0.7401 0.6369 0.3713 0.1244	0.9973 0.6369 0.8685 0.1244	0.1159 0.9925	$\begin{array}{c} 0.0091 \\ 0.0037 \\ 0.0206 \\ 0.0096 \end{array}$	0.0176 0.0037 0.0124 0.0096	0.0299 0.0000 0.0191 0.0158	0.019 0.002 0.017 0.012	0.633 0.222 0.523 0.333			
Fe2 Fe3 Fe4 O1	80 4a 8b 4a 8b	0.7401 0.6369 0.3713 0.1244 0.6112	$\begin{array}{c} 0.9973 \\ 0.6369 \\ 0.8685 \\ 0.1244 \\ 0.8733 \end{array}$	0.1159 0.9925 0.9886	0.0091 0.0037 0.0206 0.0096 0.2206	0.0176 0.0037 0.0124 0.0096 0.1421	0.0299 0.0000 0.0191 0.0158 0.0314	0.019 0.002 0.017 0.012 0.131	0.633 0.222 0.523 0.333			
Fe2 Fe3 Fe4 O1 O2	80 4a 8b 4a 8b 8b	0.7401 0.6369 0.3713 0.1244 0.6112 0.1271	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839	0.1159 0.9925 0.9886 0.9998	0.0091 0.0037 0.0206 0.0096 0.2206 0.0259	0.0176 0.0037 0.0124 0.0096 0.1421 0.0123	0.0299 0.0000 0.0191 0.0158 0.0314 0.0529	$\begin{array}{c} 0.019 \\ 0.002 \\ 0.017 \\ 0.012 \\ 0.131 \\ 0.030 \end{array}$	0.633 0.222 0.523 0.333 1 1			
Fe2 Fe3 Fe4 O1 O2 O3	80 4a 8b 4a 8b 8b 8b 8b	0.7401 0.6369 0.3713 0.1244 0.6112 0.1271 0.1253	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839 0.8802	0.1159 0.9925 0.9886 0.9998 0.0109	0.0091 0.0037 0.0206 0.0096 0.2206 0.0259 0.0618	0.0176 0.0037 0.0124 0.0096 0.1421 0.0123 0.0170	0.0299 0.0000 0.0191 0.0158 0.0314 0.0529 0.0284	$\begin{array}{c} 0.019\\ 0.002\\ 0.017\\ 0.012\\ 0.131\\ 0.030\\ 0.036\end{array}$	$\begin{array}{c} 0.633 \\ 0.222 \\ 0.523 \\ 0.333 \\ 1 \\ 1 \\ 1 \\ 1 \end{array}$			
Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4	80 4a 8b 4a 8b 8b 8b 8b 8b	0.7401 0.6369 0.3713 0.1244 0.6112 0.1271 0.1253 0.3764	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839 0.8802 0.6319	0.1159 0.9925 0.9886 0.9998 0.0109 0.9947	0.0091 0.0037 0.0206 0.0096 0.2206 0.0259 0.0618 0.0486	0.0176 0.0037 0.0124 0.0096 0.1421 0.0123 0.0170 0.0023	0.0299 0.0000 0.0191 0.0158 0.0314 0.0529 0.0284 0.0214	0.019 0.002 0.017 0.012 0.131 0.030 0.036 0.024	$\begin{array}{c} 0.633\\ 0.222\\ 0.523\\ 0.333\\ 1\\ 1\\ 1\\ 1\\ 1\end{array}$			
Fe2 Fe3 Fe4 O1 O2 O3 O4	80 4a 8b 4a 8b 8b 8b 8b 8b	0.7401 0.6369 0.3713 0.1244 0.6112 0.1271 0.1253 0.3764 80	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839 0.8802 0.6319 <i>kV (ROI-</i>)	0.1159 0.9925 0.9886 0.9998 0.0109 0.9947 1) after typ	0.0091 0.0037 0.0206 0.0096 0.2206 0.0259 0.0618 0.0486 <i>e- backgro</i>	0.0176 0.0037 0.0124 0.0096 0.1421 0.0123 0.0170 0.0023	0.0299 0.0000 0.0191 0.0158 0.0314 0.0529 0.0284 0.0214 action	0.019 0.002 0.017 0.012 0.131 0.030 0.036 0.024	0.633 0.222 0.523 0.333 1 1 1 1			
Fe2 Fe3 Fe4 O1 O2 O3 O4	80 4a 80 4a 80 80 80 80 80	$\begin{array}{c} 0.7401 \\ 0.6369 \\ 0.3713 \\ 0.1244 \\ 0.6112 \\ 0.1271 \\ 0.1253 \\ 0.3764 \\ \hline 80 \\ \delta^{-1} = 10 \end{array}$	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839 0.8802 0.6319 <i>kV (ROI-</i>	$\begin{array}{c} 0.1159\\ 0.9925\\ 0.9886\\ 0.9998\\ 0.0109\\ 0.9947\\ \hline l) after typ\\ 0 = 1.2 \\ \end{array}$	0.0091 0.0037 0.0206 0.0096 0.2206 0.0259 0.0618 0.0486 <i>e- backgro</i>	0.0176 0.0037 0.0124 0.0096 0.1421 0.0123 0.0170 0.0023 <i>pund subtra</i>	0.0299 0.0000 0.0191 0.0158 0.0314 0.0529 0.0284 0.0214 <i>action</i>	0.019 0.002 0.017 0.012 0.131 0.030 0.036 0.024	0.633 0.222 0.523 0.333 1 1 1 1			
Fe2 Fe3 Fe4 O1 O2 O3 O4	$ \begin{array}{c} 80\\ 4a\\ 8b\\ 4a\\ 8b\\ 8b\\ 8b\\ 8b\\ 8b\\ 8b\\ 8b\\ 8b\\ 8b\\ 8b$	$0.7401 \\ 0.6369 \\ 0.3713 \\ 0.1244 \\ 0.6112 \\ 0.1271 \\ 0.1253 \\ 0.3764 \\ \hline 80 \\ \textbf{\mathring{A}}^{-1} = 19;$	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839 0.8802 0.6319 <i>kV (ROI-)</i> <i>Range (Å</i>	$\begin{array}{c} 0.1159\\ 0.9925\\ 0.9886\\ 0.9998\\ 0.0109\\ 0.9947\\ \hline 0.9947\\ \hline 0.9125\\ \hline 0.9947\\ \hline 0.9125\\ \hline 0.9047\\ \hline$	0.0091 0.0037 0.0206 0.0096 0.2206 0.0259 0.0618 0.0486 <i>e- backgro</i> <i>i0; scale fa</i>	0.0176 0.0037 0.0124 0.0096 0.1421 0.0123 0.0170 0.0023 <i>pund subtra</i> <i>tetor</i> = 0.6	0.0299 0.0000 0.0191 0.0158 0.0314 0.0529 0.0284 0.0214 action i89; a (Å)	$0.019 \\ 0.002 \\ 0.017 \\ 0.012 \\ 0.131 \\ 0.030 \\ 0.036 \\ 0.024 \\ = 8.3534 \\ s^{-1} = 5$	0.633 0.222 0.523 0.333 1 1 1 1 ;			
rei Fe2 Fe3 Fe4 O1 O2 O3 O4 c (Å)	$\frac{80}{4a}$ $\frac{4a}{8b}$ $\frac{4a}{8b}$ $\frac{8b}{8b}$ $\frac{8b}{8b}$ $\frac{8b}{8b}$ $\frac{8b}{8b}$	$\begin{array}{c} 0.7401\\ 0.6369\\ 0.3713\\ 0.1244\\ 0.6112\\ 0.1271\\ 0.1253\\ 0.3764\\ \hline 80\\ \widehat{\mathbf{A}}^{-1} = 19;\\ 71; \ dampting \\ \end{array}$	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839 0.8802 0.6319 <i>kV (ROI-</i> <i>Range (Å</i> <i>ng = 0.3; a</i>	$\begin{array}{c} 0.1159\\ 0.9925\\ 0.9886\\ 0.9998\\ 0.0109\\ 0.9947\\ 1) after typ\\ 0 = 1.2 - 5\\ \delta_2 = 3.09; \end{array}$	$\begin{array}{c} 0.0091 \\ 0.0037 \\ 0.0206 \\ 0.0096 \\ \textbf{0.2206} \\ 0.0259 \\ 0.0618 \\ 0.0486 \\ \hline e \ backgree \\ \hline 0; \ scale \ fa \\ \textbf{Q}_{damp} \left(\textbf{Å}^{-1} \right) \end{array}$	$\begin{array}{c} 0.0176\\ 0.0037\\ 0.0124\\ 0.0096\\ \textbf{0.1421}\\ 0.0123\\ 0.0170\\ 0.0023\\ \hline \textbf{ound subtrative}\\ \textbf{actor} = 0.6\\ \textbf{0} = 0.0505 \end{array}$	0.0299 0.0000 0.0191 0.0158 0.0314 0.0529 0.0284 0.0214 <i>action</i> <i>89; a (Å)</i>	$\begin{array}{c} 0.019\\ 0.002\\ 0.017\\ 0.012\\ 0.131\\ 0.030\\ 0.036\\ 0.024\\ \end{array}$ $= 8.3534$ $\hat{\mathbf{A}}^{-1} = 0.$	0.633 0.222 0.523 0.333 1 1 1 1 ; ; 00457;			
rei Fe2 Fe3 Fe4 O1 O2 O3 O4 c (Å)	$ \begin{array}{c} 8b \\ 4a \\ 8b \\$	$\begin{array}{c} 0.7401 \\ 0.6369 \\ 0.3713 \\ 0.1244 \\ 0.6112 \\ 0.1271 \\ 0.1253 \\ 0.3764 \\ \hline & 80 \\ \hline & & & & \\ \hline & & & & \\ \hline & & & & \\ \hline & & & &$	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839 0.8802 0.6319 <i>kV (ROI-</i> <i>Range (Å</i> <i>ng = 0.3; a</i> <i>pdiameter</i>	$\begin{array}{c} 0.1159\\ 0.9925\\ 0.9886\\ 0.9998\\ 0.0109\\ 0.9947\\ \hline d) after typ\\ f) = 1.2 - 5\\ \delta_2 = 3.09;\\ (\AA) = 52.1 \end{array}$	$\begin{array}{c} 0.0091 \\ 0.0037 \\ 0.0206 \\ 0.0096 \\ 0.2206 \\ 0.0259 \\ 0.0618 \\ 0.0486 \\ \hline e \ backgrowth{a} \\ \hline e \ backgrowth{a} \\ \hline 0; \ scale \ fa \\ Q_{damp} (\ A^{-1} \\ 1 \ (fixed); \ delta \\ \end{array}$	$\begin{array}{c} 0.0176\\ 0.0037\\ 0.0124\\ 0.0096\\ \textbf{0.1421}\\ 0.0123\\ 0.0170\\ 0.0023\\ \hline \textbf{ound subtrative}\\ \textbf{actor} = 0.6\\ \textbf{0} = 0.0505\\ \textbf{R}_{w}(\%) = 2 \end{array}$	0.0299 0.0000 0.0191 0.0158 0.0314 0.0529 0.0284 0.0214 <i>action</i> (89; a (Å) 4; Q _{broad} (Å)	$\begin{array}{c} 0.019\\ 0.002\\ 0.017\\ 0.012\\ 0.131\\ 0.030\\ 0.036\\ 0.024\\ \hline = 8.3534\\ \mathring{\mathbf{A}}^{-1} = 0. \end{array}$	0.633 0.222 0.523 0.333 1 1 1 ; ; 00457;			
Fe2 Fe3 Fe4 O1 O2 O3 O4 c (Å)	$\frac{80}{4a}$ $\frac{4a}{8b}$ $\frac{4a}{8b}$ $\frac{8b}{8b}$ $8b$	$0.7401 0.6369 0.3713 0.1244 0.6112 0.1271 0.1253 0.3764 80 \hat{\mathbf{A}}^{-1} = 19;71; dampinspx$	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839 0.8802 0.6319 <i>kV (ROI-J</i> <i>Range (Å</i> <i>ng = 0.3; codiameter</i> <i>y</i>	$\begin{array}{c} 0.1159\\ 0.9925\\ 0.9886\\ 0.9998\\ 0.0109\\ 0.9947\\ \hline l) after typ\\ \hline l = 1.2 - 5\\ \delta_2 = 3.09;\\ \hline (A) = 52.1\\ \hline z \end{array}$	$\begin{array}{c} 0.0091 \\ 0.0037 \\ 0.0206 \\ 0.0296 \\ 0.0259 \\ 0.0618 \\ 0.0486 \\ e \ backgroup \\ e \ backgroup \\ for scale fa \\ \end{tabular} \\ \end{tabular} \\ \begin{array}{c} 0, scale fa \\ \end{tabular} \\ \end{tabular} \\ \end{tabular} \\ \begin{array}{c} 0, scale fa \\ \end{tabular} \\ \end{tabular} \\ \end{tabular} \\ \begin{array}{c} 1 \ (fixed); \\ \end{tabular} \\ \end{tabular} \end{array}$	$\begin{array}{c} 0.0176\\ 0.0037\\ 0.0124\\ 0.0096\\ \textbf{0.1421}\\ 0.0123\\ 0.0170\\ 0.0023\\ \hline \textbf{ound subtraction}\\ \textbf{out or } = 0.6\\ \textbf{0} = 0.0505\\ \textbf{R}_w(\%) = 2\\ \hline \textbf{U}_{22} \end{array}$	0.0299 0.0000 0.0191 0.0158 0.0314 0.0529 0.0284 0.0214 <i>action</i> <i>(89; a (Å)</i> <i>(4; Q_{broad} (x))</i> <i>(21.06</i> <i>U</i> 33	$0.019 \\ 0.002 \\ 0.017 \\ 0.012 \\ 0.131 \\ 0.030 \\ 0.036 \\ 0.024 \\ \hline = 8.3534 \\ \mathbf{\mathring{A}}^{-1} = 0. $	0.633 0.222 0.523 0.333 1 1 1 1 ; 00457; S.O.F.			
Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 c (Å) Fe1	$\frac{80}{4a}$ $\frac{4a}{8b}$ $\frac{4a}{8b}$ $\frac{8b}{8b}$ $\frac{8b}{8b}$ $\frac{8b}{8b}$ $\frac{8b}{8b}$	$0.7401 0.6369 0.3713 0.1244 0.6112 0.1271 0.1253 0.3764 80 \hat{\mathbf{A}}^{-1}) = 19;71; dampinspx0.7375$	0.9973 0.6369 0.8685 0.1244 0.8733 0.3839 0.8802 0.6319 <i>kV (ROI-L</i> Range (Å ng = 0.3; <i>a</i> odiameter y 0.9934	$\begin{array}{c} 0.1159\\ 0.9925\\ 0.9886\\ 0.9998\\ 0.0109\\ 0.9947\\ \hline l) after typ\\ 0 = 1.2 - 5\\ \delta_2 = 3.09;\\ (\rat{A}) = 52.1\\ \hline z\\ \hline 0.1159\end{array}$	$\begin{array}{c} 0.0091 \\ 0.0037 \\ 0.0206 \\ 0.0206 \\ 0.0259 \\ 0.0618 \\ 0.0486 \\ e \ backgrowth{a} \\ e \ backgrowth{b} \\ c \ backgrowth{b$	$\begin{array}{c} 0.0176\\ 0.0037\\ 0.0124\\ 0.0096\\ \textbf{0.1421}\\ 0.0123\\ 0.0170\\ 0.0023\\ \hline \textbf{ound subtrative}\\ \textbf{actor} = 0.6\\ \textbf{0} = 0.0505\\ \textbf{R}_w(\%) = 2\\ \hline \textbf{U}_{22}\\ \hline 0.0150 \end{array}$	$\begin{array}{c} 0.0299\\ 0.0000\\ 0.0191\\ 0.0158\\ \textbf{0.0314}\\ 0.0529\\ 0.0284\\ 0.0214\\ \hline action\\ \hline & & & \\ \hline & & \\ \hline & & \\ \hline & & \\ \hline & & \\ & & \\ \hline & & \\ \hline & & \\ & & \\ \hline & & \\ \hline & & \\ & & \\ \hline & & \\ \hline & & \\ & & \\ \hline \hline & & \\ \hline \hline & & \\ \hline & & \\ \hline \hline & & \\ \hline \hline \\ \hline & & \\ \hline \hline \\ \hline & & \\ \hline \hline \\ \hline \hline \\ \hline \\$	$\begin{array}{c} 0.019\\ 0.002\\ 0.017\\ 0.012\\ 0.131\\ 0.030\\ 0.036\\ 0.024\\ \hline \\ \hline$	0.633 0.222 0.523 0.333 1 1 1 1 ; 00457; S.O.F. 0.647			

0.9969 0.0169

Fe3

8b

0.3677

0.8655

0.0070

0.0192 0.014

0.522

Fo4	10	0 1 2 0 1	0 1 2 0 1		0.0060	0.0060	0 0000	0.007	0 333	
01	та Qh	0.1271	0.1271	0.0856	0.0000	0.0000	0.0077	0.007	0.555	
	00	0.0149	0.0015	0.9650	0.0054	0.0295	0.0951	0.003	1	
02	00	0.1108	0.5/14	0.9852	0.0132	0.0170	0.0558	0.025	1	
03	8D	0.1239	0.8040	0.015/	0.0093	0.0131	0.0184	0.014	1	
04	86	0.3/18	0.6139	0.98/6	0.0311	0.0129	0.0113	0.018	1	
300 kV (ROL 2)										
	0 ($(4^{-1}) = 19$	Range (Å	$r^{2} = 1.2 - 5$	0: scale fo	actor = 0.7	'59∙ a (Å)	= 8 3540		
(8)		· / · · ,	11411ge (11	s 240	a , setting f^{-1}			g-1	,	
С (А)	= 8.280	ss; aampi	ng = 0.4; a	$b_2 = 2.49;$	$\mathcal{Q}_{damp}(A)$) = 0.0410	$0; \boldsymbol{\mathcal{Q}}_{broad}$	4) = 0 .	00047;	
		sp	odiameter	(A) = 52.1	I (fixed);	$\boldsymbol{R}_{\boldsymbol{w}}(\boldsymbol{\%}) = I$	1.30			
Atom	Site	x	У	z	<i>U</i> ₁₁	U_{22}	U_{33}	U_{iso}	S.O.F.	
Fe1	8b	0.7541	0.9950	0.1152	0.0094	0.0237	0.0254	0.020	0.659	
Fe2	4a	0.6326	0.6326		0.0153	0.0153	0.0179	0.016	0.628	
Fe3	8b	0.3732	0.8663	0.9877	0.0114	0.0084	0.0074	0.009	0.341	
Fe4	4a	0.1325	0.1325		0.0070	0.0070	0.0433	0.019	0.333	
01	8b	0.6434	0.8708	0.9919	0.0091	0.0397	0.0087	0.019	1	
02	8b	0.1192	0.3778	1.0029	0.0090	0.0202	0.0290	0.019	1	
03	8b	0.1234	0.8792	0.0214	0.0356	0.0472	0.0038	0.029	1	
O4	8b	0.3881	0.6318	0.9740	0.0562	0.0112	0.0203	0.029	1	
		80 .	kV (ROI-2) after type	e-A backgr	ound subtr	action			
	Q_{max}	Å ⁻¹) = 19;	Range (Å) = 1.2 - 5	0; scale fa	<i>actor</i> = 0.6	62; a (Å)	= 8.3499	, ,	
c (Å)	= 8.300)9: dampi i	ng = 0.4:	$\delta_2 = 3.16$:	0 . $(Å^{-1})$) = 0.0472	8: 0 ($\mathbf{\mathring{4}}^{-1}$) = 0.	00087:	
$c(A) = 8.3009; \ damping = 0.4; \ \delta_2 = 3.16; \ Q_{damp}(A) = 0.04728; \ Q_{broad}(A^{-}) = 0.00087;$ sodiam etar $(A) = 52.11 \ (fixed); \ P \ (9/2) = 10.16$										
		sp	odiameter	(Å) = 52.1	1 (fixed); .	$R_w(\%) = I$	9.16			
Atom	Site	sp x	odiameter y	$\frac{(A) = 52.1}{z}$	$\frac{1 \text{ (fixed); }}{U_{11}}$	$\frac{R_w(\%) = 1}{U_{22}}$	19.16 U ₃₃	U _{iso}	S.O.F.	
Atom Fe1	Site 8b	<i>x</i> 0.7426	odiameter <u>y</u> 0.9992	$\frac{(A) = 52.1}{z}$	<i>l (fixed); L</i> <i>U</i> ₁₁ 0.0143	$\frac{R_w(\%) = 1}{U_{22}}$ 0.0137	$\frac{U_{33}}{U_{33}}$	U _{iso} 0.018	S.O.F. 0.597	
Atom Fe1 Fe2	Site 8b 4a	<i>x</i> 0.7426 0.6377	<i>y</i> 0.9992 0.6377	$\frac{(A) = 52.1}{z}$ 0.1130	<i>l (fixed);</i> <i>U</i> ₁₁ 0.0143 0.0111	$\frac{R_w(\%) = 1}{\frac{U_{22}}{0.0137}}$	19.16 U ₃₃ 0.0251 0.0160	U _{iso} 0.018 0.013	S.O.F. 0.597 0.450	
Atom Fe1 Fe2 Fe3	Site 8b 4a 8b	<i>x</i> 0.7426 0.6377 0.3676	y 0.9992 0.6377 0.8721	$\frac{(\hat{A}) = 52.1}{z}$ 0.1130 0.9887	<i>l (fixed); .</i> <i>U</i> ₁₁ 0.0143 0.0111 0.0139	$\frac{R_w(\%) = 1}{\frac{U_{22}}{0.0137}}$ 0.0111 0.0124	Ug.16 U33 0.0251 0.0160 0.0082	U _{iso} 0.018 0.013 0.012	S.O.F. 0.597 0.450 0.439	
Atom Fe1 Fe2 Fe3 Fe4	Site 8b 4a 8b 4a	<i>x</i> 0.7426 0.6377 0.3676 0.1247	y 0.9992 0.6377 0.8721 0.1247	$\frac{(\hat{A}) = 52.1}{z}$ 0.1130 0.9887	<i>l (fixed);</i> <i>U</i> ₁₁ 0.0143 0.0111 0.0139 0.0100	$\frac{R_w(\%) = 1}{\frac{U_{22}}{0.0137}}$ $\frac{0.0111}{0.0124}$ 0.0100	U9.16 U33 0.0251 0.0160 0.0082 0.0171	U _{iso} 0.018 0.013 0.012 0.012	S.O.F. 0.597 0.450 0.439 0.333	
Atom Fe1 Fe2 Fe3 Fe4 O1	Site 8b 4a 8b 4a 8b	<i>x</i> 0.7426 0.6377 0.3676 0.1247 0.6102	y 0.9992 0.6377 0.8721 0.1247 0.8681	$\frac{(\hat{A}) = 52.1}{z}$ 0.1130 0.9887 0.9913	$\begin{array}{c} 1 \ (fixed); \\ \hline U_{11} \\ \hline 0.0143 \\ 0.0111 \\ 0.0139 \\ 0.0100 \\ 0.0601 \end{array}$	$\frac{R_w(\%) = 1}{\frac{U_{22}}{0.0137}}$ $\frac{0.0111}{0.0124}$ 0.0100 0.0519	U9.16 U33 0.0251 0.0160 0.0082 0.0171 0.0097	U _{iso} 0.018 0.013 0.012 0.012 0.041	S.O.F. 0.597 0.450 0.439 0.333 1	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2	Site 8b 4a 8b 4a 8b 8b 8b	x 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835	$\frac{(\hat{A}) = 52.1}{z}$ 0.1130 0.9887 0.9913 1.0009	l (fixed); . U ₁₁ 0.0143 0.0111 0.0139 0.0100 0.0601 0.0259	$\frac{R_{w}(\%) = 1}{\frac{U_{22}}{0.0137}}$ $\frac{0.0111}{0.0124}$ $\frac{0.0100}{0.0519}$ 0.0177	U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049	U _{iso} 0.018 0.013 0.012 0.012 0.041 0.016	S.O.F. 0.597 0.450 0.439 0.333 1 1	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3	Site 8b 4a 8b 4a 8b 8b 8b 8b	x 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830	$\frac{(\hat{A}) = 52.1}{z}$ 0.1130 0.9887 0.9913 1.0009 0.0153	<i>l (fixed); .</i> <i>U</i> ₁₁ 0.0143 0.0111 0.0139 0.0100 0.0601 0.0259 0.4744	$\frac{R_{w}(\%) = 1}{\frac{U_{22}}{0.0137}}$ $\frac{0.0111}{0.0124}$ $\frac{0.0100}{0.0519}$ $\frac{0.0177}{0.1128}$	U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0830	U _{iso} 0.018 0.013 0.012 0.012 0.041 0.016 0.223	S.O.F. 0.597 0.450 0.439 0.333 1 1 1 1	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4	Site 8b 4a 8b 4a 8b 8b 8b 8b 8b	x 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361	$\frac{(\hat{A}) = 52.1}{z}$ 0.1130 0.9887 0.9913 1.0009 0.0153 1.0019	I (fixed); U11 0.0143 0.0111 0.0139 0.0100 0.0601 0.0259 0.4744 0.0298	$\frac{R_w(\%) = 1}{\frac{U_{22}}{0.0137}}$ $\frac{0.0111}{0.0124}$ $\frac{0.0100}{0.0519}$ $\frac{0.0177}{0.1128}$ $\frac{0.0017}{0.0017}$	U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0830 0.0421	U _{iso} 0.018 0.013 0.012 0.012 0.041 0.016 0.223 0.025	S.O.F. 0.597 0.450 0.439 0.333 1 1 1 1 1	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4	Site 8b 4a 8b 4a 8b	x 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807 80	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROL:	$\frac{(\text{\AA}) = 52.1}{\text{z}}$ 0.1130 0.9887 0.9913 1.0009 0.0153 1.0019 2) after typ	<i>l</i> (fixed); . <i>U</i> ₁₁ 0.0143 0.0111 0.0139 0.0100 0.0601 0.0259 0.4744 0.0298 <i>e- backgroupsilon</i>	$\frac{R_w(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.0017 0.0017	U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0421 action	U _{iso} 0.018 0.013 0.012 0.012 0.041 0.016 0.223 0.025	S.O.F. 0.597 0.450 0.439 0.333 1 1 1 1 1	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4	Site 8b 4a 8b 8b 8b 8b 8b 8b 8b 8b 8b	$\frac{x}{0.7426}$ 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1262 0.1502 0.3807 80 $\hat{\mathbf{A}}^{-1} = 19;$	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROI-2) Range (Å)	$\frac{(\text{\AA}) = 52.1}{z}$ 0.1130 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $1.2 - 5$	I (fixed); I U11 0.0143 0.0111 0.0139 0.0100 0.0601 0.0259 0.4744 0.0298 e- background e- background 60; scale for	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017	U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0830 0.0421 action '30; a (Å)	U_{iso} 0.018 0.013 0.012 0.012 0.041 0.016 0.223 0.025 $= 8.3566$	S.O.F. 0.597 0.450 0.439 0.333 1 1 1 1 1	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4	Site 8b 4a 8b	$\frac{x}{0.7426}$ 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807 <u>80</u> 4 ⁻¹) = 19; 28; dampin	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROI-2 Range (Å ng = 0.3; d	$\frac{(\hat{A}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$	$\frac{l (fixed);}{U_{11}}$ 0.0143 0.0111 0.0139 0.0100 0.0601 0.0259 0.4744 0.0298 e- backgro 0; scale fa Q temp (A^{-1}	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017	U_33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0830 0.0421 action '30; a (Å) 2; Q _{hman} (Å)	$ \begin{array}{r} U_{iso} \\ 0.018 \\ 0.013 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.041 \\ 0.016 \\ 0.223 \\ 0.025 \\ \hline = 8.3566 \\ 4^{-1}) = 0. \end{array} $	S.O.F. 0.597 0.450 0.439 0.333 1 1 1 ; 00909;	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 c (Å)	Site $8b$ $4a$ $8b$ $4a$ $8b$ <	$\frac{sy}{0.7426}$ 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807 80 Å ⁻¹) = 19; 28; dampin sy	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROI-2) Range (Å ng = 0.3; codiameter	$\frac{(\hat{A}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\hat{A}) = 52.1$	1 (fixed); . U ₁₁ 0.0143 0.0111 0.0139 0.0100 0.0601 0.0259 0.4744 0.0298 e-backgree i0; scale fa Q _{damp} (Å ⁻¹ 1 (fixed); .	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017	19.16 U ₃₃ 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0421 action '30; a (Å) '2; Q _{broad} (A) '9.16	$ \begin{array}{r} U_{iso} \\ 0.018 \\ 0.013 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.041 \\ 0.016 \\ 0.223 \\ 0.025 \\ = 8.3566 \\ \hat{4}^{-1}) = 0. \end{array} $	S.O.F. 0.597 0.450 0.439 0.333 1 1 1 1 ; 00909;	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 <i>c (Å)</i> Atom	Site 8b 4a 8b	$ \frac{x}{0.7426} \\ 0.7426 \\ 0.6377 \\ 0.3676 \\ 0.1247 \\ 0.6102 \\ 0.1262 \\ 0.1502 \\ 0.3807 \\ \hline 80 \\ \hline x $	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROI-2 Range (Å ng = 0.3; codiameter y	$\frac{(\mathring{A}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $2) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\mathring{A}) = 52.1$ z	$\frac{l (fixed);}{U_{11}}$ 0.0143 0.0111 0.0139 0.0100 0.0601 0.0259 0.4744 0.0298 e- backgro $i0; scale fa$ $Q_{damp}(A^{-1}$ $l (fixed);$ U_{11}	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.0017 0.0017 0.0100 0.0519 0.0418 $R_{w}(\%) = 1$ U_{22}	U33 U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0421 action '30; a (Å) 2; Qbroad (A) '29.16 U33	$ \begin{array}{r} U_{iso} \\ 0.018 \\ 0.013 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.041 \\ 0.046 \\ 0.223 \\ 0.025 \\ \hline = 8.3566 \\ \dot{A}^{-1}) = 0. \end{array} $	S.O.F. 0.597 0.450 0.333 1 1 j; 009009; S.O.F.	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 c (Å) Atom Fe1	Site 8b 4a 8b 4b 8b 8b 8b 9c max ($ae8b$	$\frac{s_{II}}{x}$ 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807 80 4 ⁻¹) = 19; 28; dampin s_{II} 28; dampin s_{II}	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROI-2 Range (Å ng = 0.3; a odiameter y 0.9959	$\frac{(\hat{A}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\hat{A}) = 52.1$ $\frac{z}{0.1114}$	$\frac{l (fixed);}{U_{11}}$ $\frac{U_{11}}{0.0143}$ 0.0111 0.0139 0.0100 0.0601 0.0259 0.4744 0.0298 $e-backgree$ $0; scale fa$ $Q_{damp}(Å^{-1}$ $l (fixed);$ $\frac{U_{11}}{0.0110}$	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.01128 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0000	$\begin{array}{c} \underline{U_{33}} \\ \hline U_{33} \\ 0.0251 \\ 0.0160 \\ 0.0082 \\ 0.0171 \\ 0.0097 \\ 0.0049 \\ 0.0830 \\ 0.0421 \\ \hline action \\ \hline 30; a (\AA) \\ 2; \ \underline{O}_{broad} (\bigstar \\ 19.16 \\ \hline U_{33} \\ 0.0133 \\ \hline \end{array}$	$ \begin{array}{r} U_{iso} \\ 0.018 \\ 0.013 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.041 \\ 0.016 \\ 0.223 \\ 0.025 \\ \hline = 8.3566 \\ \hat{4}^{-1}) = 0. \\ \hline U_{iso} \\ 0.011 \\ \hline \end{array} $	S.O.F. 0.597 0.450 0.439 0.333 1 1 ; 00909; S.O.F. 0.737	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 c (Å) Atom Fe1 Fe2	Site 8b 4a 8b 4b 8b 8b 8b 9c max(a) e 8b 4a	$\frac{s_{II}}{x}$ 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807 $\frac{80}{\text{Å}^{-1}} = 19;$ 28; dampin $\frac{s_{II}}{x}$ 0.7393 0.6382	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROI-2 Range (Å ng = 0.3; a odiameter y 0.9959 0.6382	$\frac{(\hat{A}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\hat{A}) = 52.1$ z 0.1114	$\begin{array}{r} l \ (fixed); \\ \hline U_{11} \\ \hline 0.0143 \\ 0.0111 \\ 0.0139 \\ 0.0100 \\ 0.0601 \\ 0.0259 \\ \hline 0.4744 \\ 0.0298 \\ \hline e \ backgrowth{growthmatrix} \\ e \ backgrowthmatrix \\ \hline l \ (fixed); \\ \hline U_{11} \\ 0.0110 \\ 0.0108 \\ \end{array}$	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.01128 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0001 0.0001 0.0001 0.0000 0.0000 0.0000	$\begin{array}{r} 19.16 \\ \hline U_{33} \\ 0.0251 \\ 0.0160 \\ 0.0082 \\ 0.0171 \\ 0.0097 \\ 0.0049 \\ 0.0830 \\ 0.0421 \\ \hline action \\ \hline 30; a (\AA) \\ 2; Q_{broad} (\Lambda) \\ 19.16 \\ \hline U_{33} \\ 0.0133 \\ 0.0071 \\ \end{array}$		S.O.F. 0.597 0.450 0.439 0.333 1 1 1 ; 00909; S.O.F. 0.737 0.547	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 C (Å) Atom Fe1 Fe2 Fe3	Site 8b 4a 8b 4a 8b 8b 8b 8b Site 8b 4a 8b	$\frac{s_{II}}{x}$ 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807 80 Å ⁻¹) = 19; 28; dampin s_{III} x 0.7393 0.6382 0.3659	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROL: Range (Å ng = 0.3; do odiameter y 0.9959 0.6382 0.8748	$\frac{(\hat{A}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\hat{A}) = 52.1$ $\frac{z}{0.1114}$ 0.9870	$\begin{array}{r} l \ (fixed); \\ \hline U_{11} \\ \hline 0.0143 \\ 0.0111 \\ 0.0139 \\ 0.0100 \\ 0.0601 \\ 0.0259 \\ 0.4744 \\ 0.0298 \\ \hline e \ backgrowth{a} \\ \hline 0; \ scale \ fa \\ \hline Q_{damp} \ (\AA^{-1} \\ l \ (fixed); \\ \hline U_{11} \\ \hline 0.0110 \\ 0.0108 \\ 0.0090 \\ \end{array}$	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0017 0.0001 0.0001 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000	$\begin{array}{r} 19.16 \\ \hline U_{33} \\ \hline 0.0251 \\ 0.0160 \\ 0.0082 \\ 0.0171 \\ 0.0097 \\ 0.0049 \\ \hline 0.0830 \\ 0.0421 \\ \hline action \\ \hline 30; a (\AA) \\ \hline 2; Q_{broad} (\Lambda) \\ \hline 29.16 \\ \hline U_{33} \\ \hline 0.0133 \\ 0.0071 \\ 0.0103 \\ \end{array}$		S.O.F. 0.597 0.450 0.439 0.333 1 1 1 <i>j</i> 00909; S.O.F. 0.737 0.547 0.717	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 O4 <i>c (Å)</i> Atom Fe1 Fe2 Fe3 Fe4	Site 8b 4a 8b 4b 8b 8b 8b 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 8b	$\frac{sy}{0.7426}$ 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807 80 Å ⁻¹) = 19; 28; dampin sy x 0.7393 0.6382 0.3659 0.1264	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROL: mg = 0.3; codiameter y 0.9959 0.6382 0.8748 0.1264	$\frac{(\hat{A}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\hat{A}) = 52.1$ z 0.1114 0.9870	$\begin{array}{r} l \ (fixed); \\ \hline U_{11} \\ \hline 0.0143 \\ 0.0111 \\ 0.0139 \\ 0.0100 \\ 0.0601 \\ 0.0259 \\ 0.4744 \\ 0.0298 \\ \hline e \ backgroad \\ \hline 0; \ scale \ for \\ \hline Q_{damp} \ ({\AA}^{-1} \\ \hline 1 \ (fixed); \\ \hline U_{11} \\ \hline 0.0110 \\ 0.0108 \\ 0.0090 \\ 0.0050 \\ \end{array}$	$\frac{R_w(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.0017 0.0017 0.0017 0.00448 $\frac{R_w(\%) = 1}{U_{22}}$ 0.0086 0.0108 0.0120 0.0050	$\begin{array}{r} 19.16 \\ \hline U_{33} \\ \hline 0.0251 \\ 0.0160 \\ 0.0082 \\ 0.0171 \\ 0.0097 \\ 0.0049 \\ \hline 0.0830 \\ 0.0421 \\ \hline action \\ \hline 30; a (\AA) \\ \hline 2; Q_{broad} (\Lambda) \\ \hline 23 \\ \hline 0.0133 \\ 0.0071 \\ 0.0103 \\ 0.0053 \\ \hline \end{array}$		S.O.F. 0.597 0.450 0.439 0.333 1 1 1 <i>i i i</i> 0.90909; S.O.F. 0.737 0.547 0.717 0.333	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 C (Å) Atom Fe1 Fe2 Fe3 Fe4 O1	Site 8b 4a 8b 4a 8b 8b 8b 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 8b 4a 8b	$ \begin{array}{r} sy \\ \hline x \\ 0.7426 \\ 0.6377 \\ 0.3676 \\ 0.1247 \\ 0.6102 \\ 0.1262 \\ 0.1502 \\ 0.3807 \\ \hline 80 $	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8830 0.6361 kV (ROI-2) Range (Å ng = 0.3; codiameter y 0.9959 0.6382 0.8748 0.1264 0.8731	$\frac{(\hat{A}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\hat{A}) = 52.1$ z 0.1114 0.9870 0.9901	$\begin{array}{r} l \ (fixed); \\ \hline U_{11} \\ \hline 0.0143 \\ 0.0111 \\ 0.0139 \\ 0.0100 \\ 0.0601 \\ 0.0259 \\ 0.4744 \\ 0.0298 \\ \hline e-backgree \\ \hline 0; \ scale \ fa \\ \hline 0; \ scale \ fa \\ \hline 0; \ scale \ fa \\ \hline 0, \ scale \ fa \\ \hline 0.0110 \\ 0.0108 \\ 0.0090 \\ 0.0050 \\ 0.0121 \\ \end{array}$	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.0017 0.0017 0.00448 $\frac{W_{22}}{0.0086}$ 0.0108 0.0120 0.0275	U33 U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0421 0.0421 action 30; a (Å) 2; Qbroad (A) 0.0133 0.0133 0.0071 0.0103 0.0053 0.0178 0.0178	$ \begin{array}{r} U_{iso} \\ 0.018 \\ 0.013 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.025 \\ \hline = 8.3566 \\ \dot{A}^{-1} = 0. \\ \hline U_{iso} \\ 0.011 \\ 0.010 \\ 0.010 \\ 0.005 \\ 0.019 \\ \end{array} $	S.O.F. 0.597 0.450 0.439 0.333 1 1 1 <i>i i i</i> 0.0909; S.O.F. 0.737 0.547 0.717 0.333 1	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 C (Å) Atom Fe1 Fe2 Fe3 Fe4 O1 O2	Site 8b 4a 8b 4a 8b 8b 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b 4a 8b	$\begin{array}{r} sy \\ \hline x \\ \hline 0.7426 \\ 0.6377 \\ 0.3676 \\ 0.1247 \\ 0.6102 \\ 0.1262 \\ 0.1502 \\ 0.3807 \\ \hline 80 \\ \hline$	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8681 0.36361 kV (ROI-2 Range (Å ng = 0.3; dot odiameter y 0.9959 0.6382 0.8748 0.1264 0.8731 0.3949	$\frac{(\text{\AA}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\text{\AA}) = 52.1$ z 0.1114 0.9870 0.9901 0.9958	$\frac{l (fixed);}{U_{11}}$ 0.0143 0.0111 0.0139 0.0100 0.0601 0.0259 0.4744 0.0298 e- backgro 0; scale fa Q_damp(Å^{-1} 1 (fixed); U_{11} 0.0110 0.0108 0.0090 0.0050 0.0121 0.0205	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.0017 0.0017 0.00448 $\frac{R_{w}(\%) = 1}{U_{22}}$ 0.0086 0.0108 0.0120 0.0050 0.0275 0.0138	U33 U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0421 0.0121 action 230; a (Å) 22; Qbroad (Å) 22; Qbroad (Å) 0.0133 0.0071 0.0103 0.0053 0.0178 0.0020	$ \begin{array}{r} U_{iso} \\ 0.018 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.041 \\ 0.023 \\ 0.025 \\ \hline = 8.3566 \\ \dot{A}^{-1} = 0. \\ \hline U_{iso} \\ 0.011 \\ 0.010 \\ 0.010 \\ 0.005 \\ 0.019 \\ 0.012 \\ \end{array} $	S.O.F. 0.597 0.450 0.439 0.333 1 1 1 1 5 00909; S.O.F. 0.737 0.547 0.717 0.333 1 1	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 <i>c (Å)</i> Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3	Site $8b$ $4a$ $8b$ $4a$ $8b$ $4a$ $8b$ $4a$ $8b$ $4a$ $8b$	$\frac{sy}{0.7426}$ 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807 80 4 ⁻¹) = 19; 28; dampin sy 28; dampin 59 0.7393 0.6382 0.3659 0.1264 0.6087 0.1212 0.1293	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8630 0.6361 kV (ROI-2 Range (Å ng = 0.3; codiameter y 0.9959 0.6382 0.8748 0.1264 0.8731 0.3949 0.8862	$\frac{(\text{\AA}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\text{\AA}) = 52.1$ z 0.1114 0.9870 0.9901 0.9958 0.0105	$\begin{array}{r} l \ (fixed); \\ \hline U_{11} \\ 0.0143 \\ 0.0111 \\ 0.0139 \\ 0.0100 \\ 0.0601 \\ 0.0259 \\ 0.4744 \\ 0.0298 \\ e \ backgrowth{a} \\ e \ backgrowth{a} \\ c \ backgrowth{a} \\ c$	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.0017 0.0017 0.00448 $\frac{R_{w}(\%) = 1}{U_{22}}$ 0.0086 0.0108 0.0120 0.0050 0.0275 0.0138 0.0299	U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0830 0.0421 action '30; a (Å) '2; Qbroad (A) '2, Qbroad (A) '0.103 0.0133 0.0053 0.0178 0.0020 0.0197	$ \begin{array}{r} U_{iso} \\ 0.018 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.025 \\ \hline = 8.3566 \\ \dot{4}^{-1}) = 0. \\ \hline U_{iso} \\ 0.011 \\ 0.010 \\ 0.005 \\ 0.019 \\ 0.012 \\ 0.025 \\ \end{array} $	S.O.F. 0.597 0.450 0.439 0.333 1	
Atom Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4 <i>c (Å)</i> Fe1 Fe2 Fe3 Fe4 O1 O2 O3 O4	Site $8b$ $4a$ $8b$ $4a$ $8b$ $4a$ $8b$ $4a$ $8b$ $8b$ $8b$ $8b$ $8b$ $8b$	$\frac{s_{II}}{x}$ 0.7426 0.6377 0.3676 0.1247 0.6102 0.1262 0.1502 0.3807 80 4 ⁻¹) = 19; 28; dampin s_{II} 28; dampin 0.7393 0.6382 0.3659 0.1264 0.6087 0.1212 0.1293 0.3822	y 0.9992 0.6377 0.8721 0.1247 0.8681 0.3835 0.8630 0.6361 kV (ROI-2 Range (Å ng = 0.3; c odiameter y 0.9959 0.6382 0.8748 0.1264 0.8731 0.3949 0.8862 0.6379	$\frac{(\hat{A}) = 52.1}{z}$ $\frac{z}{0.1130}$ 0.9887 0.9913 1.0009 0.0153 1.0019 $2) after typ$ $b) = 1.2 - 5$ $\delta_2 = 3.21;$ $(\hat{A}) = 52.1$ z 0.1114 0.9870 0.9901 0.9958 0.0105 1.0013	$\begin{array}{r} l \ (fixed); \\ \hline U_{11} \\ \hline 0.0143 \\ 0.0111 \\ 0.0139 \\ 0.0100 \\ 0.0601 \\ 0.0259 \\ 0.4744 \\ 0.0298 \\ \hline e \ backgrowth{a} \\ e^{-backgrowth{a}} (A^{-1} \\ I \ (fixed); \\ \hline U_{11} \\ 0.0110 \\ 0.0108 \\ 0.0090 \\ 0.0050 \\ 0.0121 \\ 0.0255 \\ 0.0130 \\ \hline \end{array}$	$\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0137}$ 0.0111 0.0124 0.0100 0.0519 0.0177 0.1128 0.0017 0.0128 0.0017 0.0448 $\frac{R_{w}(\%) = 1}{U_{22}}$ $\frac{U_{22}}{0.0086}$ 0.0108 0.0120 0.0050 0.0275 0.0138 0.0299 0.0002	U33 0.0251 0.0160 0.0082 0.0171 0.0097 0.0049 0.0421 action '30; a (Å) '2; Qbroad (Å) '9.16 U33 0.0133 0.0053 0.0178 0.0020 0.0181	$ \begin{array}{r} U_{iso} \\ 0.018 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.012 \\ 0.025 \\ \hline = 8.3566 \\ 4^{-1}) = 0. \\ \hline U_{iso} \\ 0.011 \\ 0.010 \\ 0.010 \\ 0.012 \\ 0.025 \\ 0.010 \\ 0.025 \\ 0.010 \\ \end{array} $	S.O.F. 0.597 0.450 0.439 0.333 1	

				<u>300 k</u> l	V (ROI-3)					
$Q_{max}(\dot{A}^{-1}) = 19$; Range $(\dot{A}) = 1.2 - 50$; scale factor = 0.749; a $(\dot{A}) = 8.3404$;										
$c(A) = 8.3005; damping = 0.3; \delta_2 = 2.88; O, (A^{-1}) = 0.04779; O. (A^{-1}) = 0.00121;$										
$spdiameter (Å) = 52.11 (fixed): R_{}(\%) = 11.20$										
A 4	C:4-	<u> </u>		, , , , , , , , , , , , , , , , , , ,	IT	w(70) 1 IT	1.20 II	TT.	SOF	
Atom	Site	<u>x</u>	<u>y</u>	2	U_{11}				S.O.F.	
Fel	8b	0.7410	1.0019	0.1312	0.0163	0.0122	0.0222	0.017	0.643	
Fe2	4a	0.6200	0.6200	0.0014	0.0019	0.0019	0.0044	0.003	0.174	
Fe3	8b	0.3791	0.8735	0.9914	0.0105	0.0201	0.0143	0.015	0.524	
Fe4	4a	0.1117	0.1117		0.0050	0.0050	0.0119	0.007	0.333	
01	8b	0.6216	0.8755	0.9921	0.0112	0.0301	0.0081	0.016	1	
02	8b	0.1162	0.3641	0.9642	0.0269	0.0572	0.0894	0.058	1	
03	8b	0.1166	0.8723	0.0105	0.0107	0.0284	0.0120	0.017	1	
04	8b	0.3595	0.6321	0.9771	0.0129	0.0235	0.0061	0.014	1	
		80	kV (ROI-3)) after type	e-A backgr	ound subtr	action			
	Q	$\mathbf{\hat{4}}^{-1}$) = 19;	Range (Å) = 1.2 - 5	0; scale f a	actor = 0.7	28; a (Å)	= 8.3576	;	
c (Å)	= 8.264	10. damnii	$n\sigma = 0.4 \cdot d$	$S_{2} = 2.92 \cdot 10^{-3}$	$0 (A^{-1})$) = 0.0460	1.0 ($(4^{-1}) = 0$	00882.	
C (11)	0.20	si	ndiameter	$(\mathbf{A}) = 52.1$	Z _{damp} (1 1 (fixed)	R (%) = 1	$^{1}, \mathcal{L}_{broad}$	1) 0.	00002,	
Atom	Site	<u> </u>		-	<u>I</u>	<u>II</u>	<u> </u>	I I	SOF	
Atom E.1	<u>91</u>	x	<u>y</u>	4	$\frac{U_{11}}{0.0127}$	0.0251	0.0222		5.0.F.	
Fel E.2	8D	0./301	1.0029	0.1242	0.013/	0.0251	0.0332	0.024	0.543	
Fe2	4a	0.6385	0.6385	0.0075	0.0093	0.0093	0.008/	0.009	0.353	
Fe3	86	0.368/	0.8680	0.98/5	0.00/3	0.00/6	0.0054	0.00/	0.284	
Fe4	4a	0.1255	0.1255		0.0145	0.0145	0.0104	0.013	0.333	
01	8b	0.6065	0.8432	0.9891	0.0278	3.5994	0.0236	1.217	1	
02	8b	0.1289	0.3851	1.0078	0.0281	0.0235	0.0310	0.028	l	
03	8b	0.1368	0.8692	0.0225	0.0093	0.0458	0.0297	0.028	1	
04	8b	0.3835	0.6265	0.9896	0.0288	0.0126	0.0253	0.022	1	
		80	kV (ROI-3	3) after typ	e- backgro	ound subtre	action			
	$Q_{max}(z)$	Å ⁻¹) = 19;	Range (Å) = 1.2 - 5	0; scale fa	actor = 0.6	91; a (Å)	= 8.3518	;	
c (Å)	= 8.270)6: dampi i	ng = 0.4: d	$\delta_2 = 2.80$:	$0. (Å^{-1})$) = 0.0451	5: 0 ($(4^{-1}) = 0.$	00106:	
		SL.	odiameter	(A) = 52.1	1 (fixed);	$R_w(\%) = 1$	9.63	,	,	
Atom	Site	x	y	z	U_{11}	U ₂₂	U_{33}	Uiso	S.O.F.	
Fe1	8b	0.7517	0.9937	0.1123	0.0148	0.0141	0.0289	0.019	0.665	
Fe2	4a	0.6312	0.6312		0.0173	0.0173	0.0140	0.016	0.626	
Fe3	8b	0.3655	0.8740	0.9892	0.0049	0.0100	0.0148	0.010	0.349	
Fe4	4a	0.1292	0.1292	J., U, Z	0.0137	0.0137	0.0079	0.012	0.333	
01	8b	0.6269	0.8490	0.9803	0.0287	0.0563	0.0010	0.029	1	
02	8b	0.1169	0.3913	1.0076	0.0180	0.0080	0.0146	0.014	1	
03	8b	0 1 1 9 3	0.8695	0.0094	0.0464	0.0369	0.0362	0.040	1	
04	8b	0.3818	0.6333	0.9867	0.0306	0.0035	0.0127	0.016	1	

				300 kl	V (ROI-4)						
	$Q_{max}(\dot{A}^{-1}) = 19$; Range $(\dot{A}) = 1.2 - 50$; scale factor = 0.845; a $(\dot{A}) = 8.3480$;										
$c(\mathbf{A}) = 8.2979; \ damping = 0.4; \ \delta_2 = 2.95; \ O_1 = (\mathbf{A}^{-1}) = 0.04394; \ O_2 = 0.00118;$											
spdiameter $(\mathring{A}) = 52.11$ (fixed); $R_w(\%) = 11.70$											
Atom	Sito	- <u>-</u> r	17	7	I I	<u> </u>	U	U.	SOF		
Fol	86	0 7326	<u> </u>	<u> </u>	0.0330	0.0087	0.0152	0.010	0.670		
Fel	80 49	0.7320	0.6389	0.1202	0.0330	0.0087	0.0132	0.019	0.079		
Fe2 Fo3	7a 8h	0.0589	0.0389	0 0860	0.0113	0.0119	0.0143	0.015	0.505		
Fe4	49	0.1228	0.0729	0.7007	0.0213	0.0157	0.0112	0.010	0.303		
01	4a 8b	0.1228	0.1228	0 9646	0.0034	0.0004	0.0124	0.008	0.355		
$\frac{01}{02}$	8b	0.1167	0.3852	0.9040	0.0790	0.0000	0.0100	0.012	1		
02	8b	0.1531	0.3632	0.0255	0.0075	0.0105	0.0174	0.012	1		
04	8b	0.3898	0.6007	0.0255	0.0103	0.0120	0.0079	0.030	1		
	00	80	kV (ROI-4) after type	-A hacker	ound subtr	action	0.012			
	0 ($(a^{-1}) = 10$	Range (Å	(-1) = 12 - 5	1) scale f	actor = 0.5	87: a (Å)	= 8 3510			
	$\mathcal{L}_{max}(2)$	1 <i>)</i> 1), 75. damai	$\mathbf{A} = 0.2$	1.2 - 3	O, scale fi	$(0.01 \ 0.5)$	67, u (A)	(1) = 0	, 000 <i>44</i> .		
С (А)	= 8.277	/s; aampii	ng = 0.3; a	$b_2 = 3.20;$	$\mathcal{Q}_{damp}(A)$) = 0.0515	$0; \boldsymbol{\mathcal{Q}}_{broad}$	4) = 0 .	00044;		
. <u></u>		sp	balameter	(A) = 52.1	1 (fixea);	$K_w(\%) = 2$	20.30				
Atom	Site	x	У	z	U_{11}	U_{22}	U_{33}	U_{iso}	S.O.F.		
Fe1	8b	0.7397	0.9987	0.1193	0.0142	0.0152	0.0225	0.017	0.597		
Fe2	4a	0.6377	0.6377		0.0099	0.0099	0.0024	0.007	0.287		
Fe3	8b	0.3708	0.8699	0.9879	0.0135	0.0092	0.0103	0.011	0.457		
Fe4	4a	0.1237	0.1237		0.0106	0.0106	0.0113	0.011	0.333		
01	8b	0.5989	0.8755	0.9681	0.3188	0.1068	0.1948	0.207	1		
02	8b	0.1125	0.3755	0.9778	0.0078	0.0277	0.0302	0.022	1		
03	8b	0.1297	0.8644	0.0104	0.0273	0.0255	0.0155	0.023	1		
04	8b	0.3787	0.6179	0.9906	0.0205	0.0094	0.0104	0.013	1		
		80	kV (ROI-4	!) after typ	e- backgro	ound subtra	action				
	Q_{max}	Å ⁻¹) = 19;	Range (Å) = 1.2 - 5	0; scale f a	<i>actor</i> = 0.6	10; a (Å)	= 8.3560	;		
c (Å)	= 8.273	34; dampi i	ng = 0.4; d	$b_2 = 3.17;$	$Q_{damm}(\AA^{-1}$) = 0.0519	3; Q _{broad} ($\mathbf{\mathring{A}}^{-1}$) = θ .	00307;		
		sp	odiameter	(Å) = 52.1	1 (fixed);	$R_w(\%) = 2$	22.07				
Atom	Site	x	у	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.		
Fe1	8b	0.7392	1.0046	0.1271	0.0161	0.0139	0.0224	0.017	0.658		
Fe2	4a	0.6255	0.6255		0.0161	0.0161	0.0101	0.014	0.432		
Fe3	8b	0.3675	0.8703	0.9868	0.0132	0.0125	0.0096	0.012	0.490		
Fe4	4a	0.1304	0.1304		0.0058	0.0058	0.0180	0.010	0.333		
01	8b	0.6225	0.8687	0.9908	0.0330	0.0112	0.0166	0.020	1		
02	8b	0.1149	0.3823	0.9907	0.0215	0.0424	0.0673	0.044	1		
03	8b	0.1363	0.8772	0.0064	0.0751	0.0379	0.0155	0.043	1		
04	8b	0.3737	0.6272	0.9908	0.0329	0.0170	0.0428	0.031	1		

300 kV (ROI-5)												
$Q_{mm}(A^{-1}) = 19$; Range $(A) = 1.2 - 50$; scale factor = 0.726; a $(A) = 8.3433$:												
$c(\mathbf{A}) = 8.2986$; damping = 0.3; $\delta_2 = 3.04$; 0 $(\mathbf{A}^{-1}) = 0.04771$; 0 $(\mathbf{A}^{-1}) = 0.00426$.												
sndiameter $(\hat{A}) = 52 11$ (fixed): $R_{}(\mathcal{A}) = 11 71$												
Atom Site v v a U U U U SOF												
Atom E.1	Site	<i>x</i>	<u>y</u>	<u><u></u> 0 11(1</u>	$\frac{U_{11}}{0.0000}$	$\frac{U_{22}}{0.0219}$	$\frac{U_{33}}{0.0124}$	U_{iso}	5.U.F.			
rei Es2	80 40	0.7441 0.6200	0.9928	0.1101	0.0090	0.0218	0.0124	0.014	0.703			
rez Es2	4a 01	0.0309	0.0309	0.0000	0.0122	0.0122	0.0505	0.020	0.007			
res Esd	40	0.3030	0.8/20 0.1275	0.9900	0.0055	0.0101	0.0170	0.010	0.4//			
ге4	4a 01	0.15/5	0.15/5	0.0022	0.0213	0.0213	0.0190	0.021	0.555			
	00 91	0.0202	0.80/5	0.9833	0.0239	0.0143	0.0540	0.023	1			
02	00 91	0.0997	0.3044	0.9652	0.0031	0.0130	0.0155	0.011	1			
03	80 86	0.11/9	0.6021	0.0040	0.0185	0.0221	0.0043	0.013	1			
04	80	0.3701	0.0330	0.9910	0.0079	0.0139	0.0213	0.014	1			
80 kV (KOI-5) after type-A background subtraction												
$Q_{max}(A^{-1}) = 19$; Range $(A) = 1.2 - 50$; scale factor = 0.568; a $(A) = 8.3578$;												
c (Å)	= 8.284	45; <mark>dampi</mark> l	ng = 0.4; d	$\delta_2 = 3.17;$	$Q_{damn}(\AA^{-1})$) = 0.0476	3; Q _{broad} (2	$\mathbf{\mathring{4}}^{-1}) = 0.$	00676;			
spdiameter (Å) = 52.11 (fixed); R_w (%) = 22.31												
Atom	Site	x	v	z	U_{11}	U_{22}	U_{33}	Uiso	S.O.F.			
Fe1	8b	0.7394	1.0000	0.1106	0.0155	0.0154	0.0265	0.019	0.756			
Fe2	4a	0.6235	0.6235		0.0315	0.0315	0.0186	0.027	1.059			
Fe3	8b	0.3684	0.8678	0.9912	0.0053	0.0120	0.0099	0.009	0.334			
Fe4	4a	0.1327	0.1327		0.0026	0.0026	0.0244	0.010	0.333			
01	8b	0.6178	0.8524	0.9963	0.0239	0.1658	0.0125	0.067	1			
02	8b	0.1179	0.3962	0.9974	0.0142	0.0151	0.0276	0.019	1			
03	8b	0.1199	0.8869	0.0168	0.0798	0.0000	0.0110	0.030	1			
04	8b	0.3668	0.6267	0.9890	0.0073	0.0084	0.0237	0.013	1			
		80	kV (ROI-5	5) after typ	e- backgro	ound subtra	action					
	0 ($\mathbf{\hat{4}}^{-1}$) = 19:	Range (Å) = 1.2 - 5	0: scale fo	actor = 0.6	72: a (Å)	= 8.3554	÷			
c (Å)	- max \ = 8 289	85 · damni	$n \sigma = 0.4 \cdot \lambda$	$5_{2} - 3.01$	$0 (l^{-1})$) = 0.0458	$0 \cdot 0 ($	$(h^{-1}) = 0$, nnn20.			
C (A)	- 0.200	s, uumpu	ng 0.7, 0 Ndiam <i>ete</i> r	$(\mathbf{A}) = 521$	$\mathcal{L}_{damp}(A)$	R (%) = 1), D _{broad} (2 18 93	1) 0.	00027,			
Atom	Sito	şı 	,	-	<u>I (Jineu), i</u>	$\frac{n_w(70)}{17}$	0.75 II	I I	SOF			
Fo1	Site 9h	<i>x</i>	<u> </u>	<u> </u>	$\frac{U_{11}}{0.0081}$	$\frac{U_{22}}{0.0122}$	$\frac{U_{33}}{0.0201}$	$\frac{U_{iso}}{0.017}$	5.0.F .			
Fel Fol	40	0.7399	0.6222	0.1124	0.0081	0.0155	0.0291	0.017	0.009			
ге2 Ба2	4a 8h	0.0352	0.0352	0 0800	0.0101	0.0101	0.0244	0.019	0.077			
гез Ба4	00 /0	0.3004	0.0712	0.2029	0.0127	0.009/	0.0043	0.009	0.377			
г с 4 01	4a 8h	0.1200	0.1200	0 9801	0.0108	0.0108	0.0000	0.009	0.555			
	8b	0.0213	0.8050	1 0012	0.0310	0.0155	0.0213	0.023 0.017	1			
02	00 8h	0.1225	0.3004	0.0107	0.0292	0.0104	0.0000	0.017	1			
03	00 81	0.1500	0.0042	0.019/	0.0322	0.0044	0.0442	0.000	1			
04	ðD	0.3/04	0.0330	0.9952	0.0414	0.0108	0.0313	0.030	1			

300 kV (ROI-6)											
0 $(\mathring{A}^{-1}) = 19$: Range $(\mathring{A}) = 1.2 - 50$: scale factor = 0.794: a $(\mathring{A}) = 8.3451$:											
$z_{max}(x^2) = 0.25 + 2.8 + 2.82 + 0.04642 + 0.04642 + 0.00200$											
$c_{(A)} = 0.2900, \text{ aumping} = 0.3, o_2 = 2.03, \mathcal{Q}_{damp}(A_{-}) = 0.004042, \mathcal{Q}_{broad}(A_{-}) = 0.00290,$											
spliameter (A) = 52.11 (fixed); R_w (%) = 13.05											
Atom	Site	x	у	z	<i>U</i> ₁₁	U_{22}	U_{33}	U _{iso}	S.O.F.		
Fe1	8b	0.7461	0.9986	0.1118	0.0108	0.0107	0.0341	0.019	0.686		
Fe2	4a	0.6354	0.6354		0.0156	0.0156	0.0178	0.016	0.720		
Fe3	8b	0.3685	0.8697	0.9878	0.0104	0.0114	0.0040	0.009	0.301		
Fe4	4a	0.1237	0.1237		0.0103	0.0103	0.0115	0.011	0.333		
01	8b	0.6420	0.8821	0.9719	0.0222	0.0278	0.0043	0.018	1		
02	8b	0.1217	0.3777	0.9979	0.0217	0.0161	0.0166	0.018	1		
03	8b	0.1483	0.8743	0.0251	0.0211	0.0215	0.0092	0.017	1		
O4	8b	0.3817	0.6274	0.9931	0.0153	0.0174	0.0162	0.016	1		
80 kV (ROI-6) after type-A background subtraction											
$Q_{max}(\dot{A}^{-1}) = 19$; Range $(\dot{A}) = 1.2 - 50$; scale factor = 0.647; a $(\dot{A}) = 8.3489$;											
c (Å)	= 8.274	41; dampi i	ng = 0.4; d	$\delta_2 = 3.21;$	0 ,(Å ⁻¹) = 0.0527	2; 0 ,	$\mathbf{\mathring{A}}^{-1}$) = θ .	00421;		
spdiameter $(A) = 52.11$ (fixed); $R_w(\%) = 18.50$											
Atom	Site	x	у	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.		
Fe1	8b	0.7411	1.0028	0.1127	0.0098	0.0153	0.0308	0.019	0.534		
Fe2	4a	0.6367	0.6367		0.0155	0.0155	0.0023	0.011	0.341		
Fe3	8b	0.3696	0.8685	0.9996	0.0159	0.0146	0.0217	0.017	0.416		
Fe4	4a	0.1202	0.1202		0.0072	0.0072	0.0227	0.012	0.333		
01	8b	0.5642	0.9484	0.9420	0.1559	4.8663	0.0955	1.706	1		
02	8b	0.1092	0.3763	0.9807	0.0054	0.0241	0.0563	0.029	1		
03	8b	0.1241	0.8690	0.0107	0.0347	0.0517	0.0231	0.037	1		
O4	8b	0.3775	0.6156	0.9940	0.0197	0.0199	0.0164	0.019	1		
		80	kV (ROI-0	6) after typ	e- backgro	ound subtre	action				
	Q_{max}	$\mathbf{\mathring{A}}^{-1}$) = 19;	Range (Å) = 1.2 - 5	0; scale f a	actor = 0.5	511; a (Å)	= 8.3583	;		
c (Å)	= 8.260	54: dampi i	ng = 0.3:	$\delta_2 = 3.07$:	0 . $(Å^{-1})$) = 0.0517	71: 0 ($(\dot{A}^{-1}) = 0.$	00572:		
spdiameter $(A) = 52.11$ (fixed); $R_w(\%) = 25.06$											
Atom	Site	x	у	z	<i>U</i> ₁₁	U ₂₂	U ₃₃	U _{iso}	S.O.F.		
Fe1	8b	0.7408	0.9967	0.1178	0.0153	0.0096	0.0247	0.017	0.685		
Fe2	4a	0.6351	0.6351		0.0100	0.0100	0.0049	0.008	0.315		
Fe3	8b	0.3709	0.8704	0.9879	0.0119	0.0151	0.0048	0.011	0.556		
Fe4	4a	0.1183	0.1183		0.0063	0.0063	0.0045	0.006	0.333		
01	8b	0.6158	0.8642	0.9887	0.0031	0.0141	0.0233	0.014	1		
02	8b	0.1170	0.3843	1.0000	0.0100	0.0221	0.0075	0.013	1		
03	8b	0.1434	0.8731	0.0153	0.0120	0.0345	0.0890	0.045	1		
04	<u>8</u> b	0.3762	0.6277	0.9944	0.0198	0.0621	0.0112	0.031	1		

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