FOUNDATIONS
ADVANCES

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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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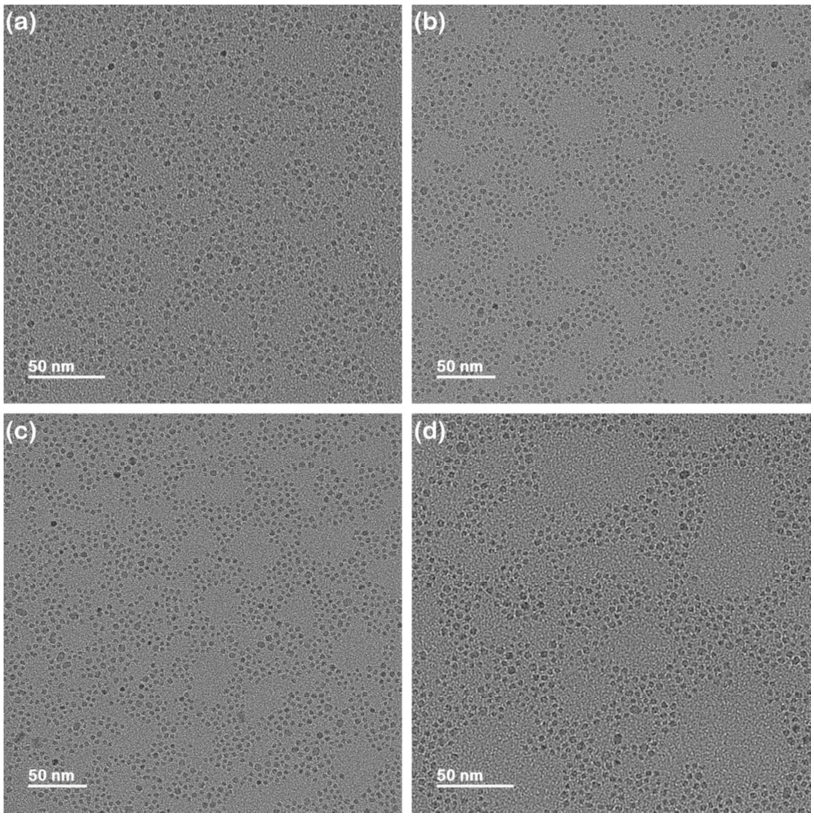

Figure S1 TEM bright field images of dispersed as-synthesized nanoparticles showing the spherical morphology.

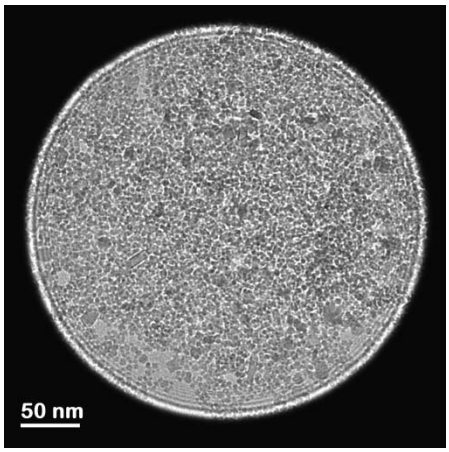

Figure S2 Illumination of agglomerated as-synthesized nanoparticles using a parallel probe formed by 50 μm condenser aperture.

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 ($2P_{1/2}$ and $2P_{3/2}$) to unoccupied 3d levels show characteristic L_3 and L_2 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 L_3 and L_2 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.

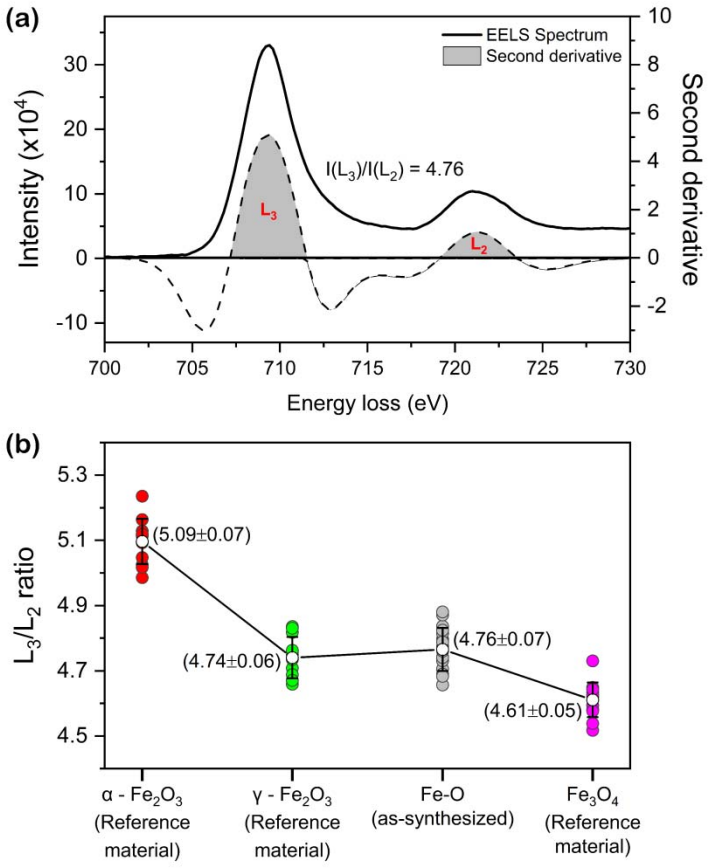

Figure S3 Comparison of EELS White Lines Ratio (WLR) obtained from as-synthesized and standard reference iron oxide nanoparticles. (a) illustrates the positive contribution of Fe-L_3 and L_2 peaks after the second derivative of intensities acquired from one of the regions of interest (ROI) of as-synthesized nanoparticles. The WLR is performed from various ROIs' and represented by a circle filled with red (α-Fe_2O_3 std.), green (γ-Fe_2O_3 std.), grey (as-synthesized), and magenta (Fe_3O_4 std.)

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

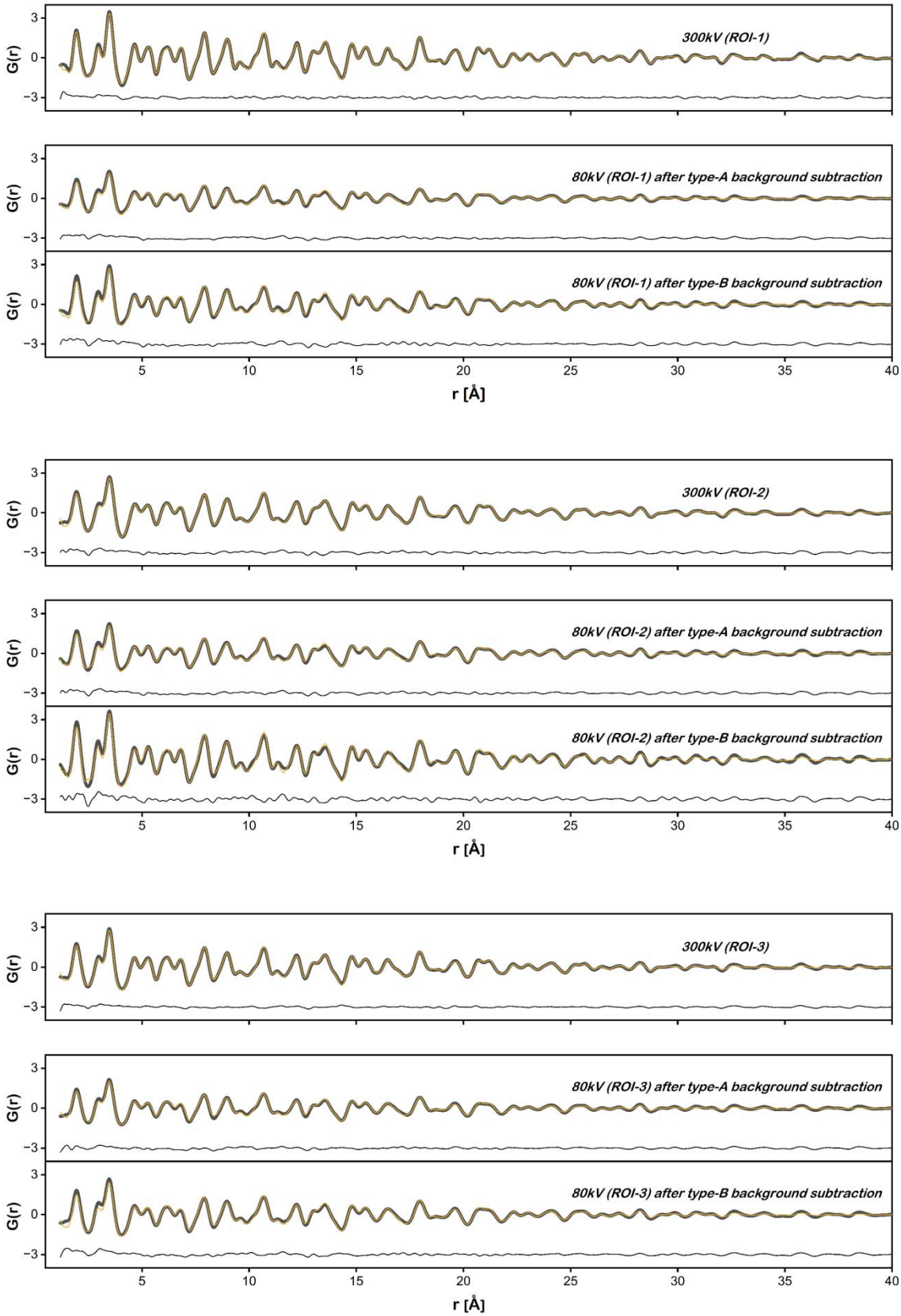

Figure S4 Comparison of refined e-PDF $G(r)$ profiles obtained at various regions of interest (ROI) using 300 kV and 80 kV electron beam energy. Related $\phi(q)$ profiles were overlaid in Fig. 6.

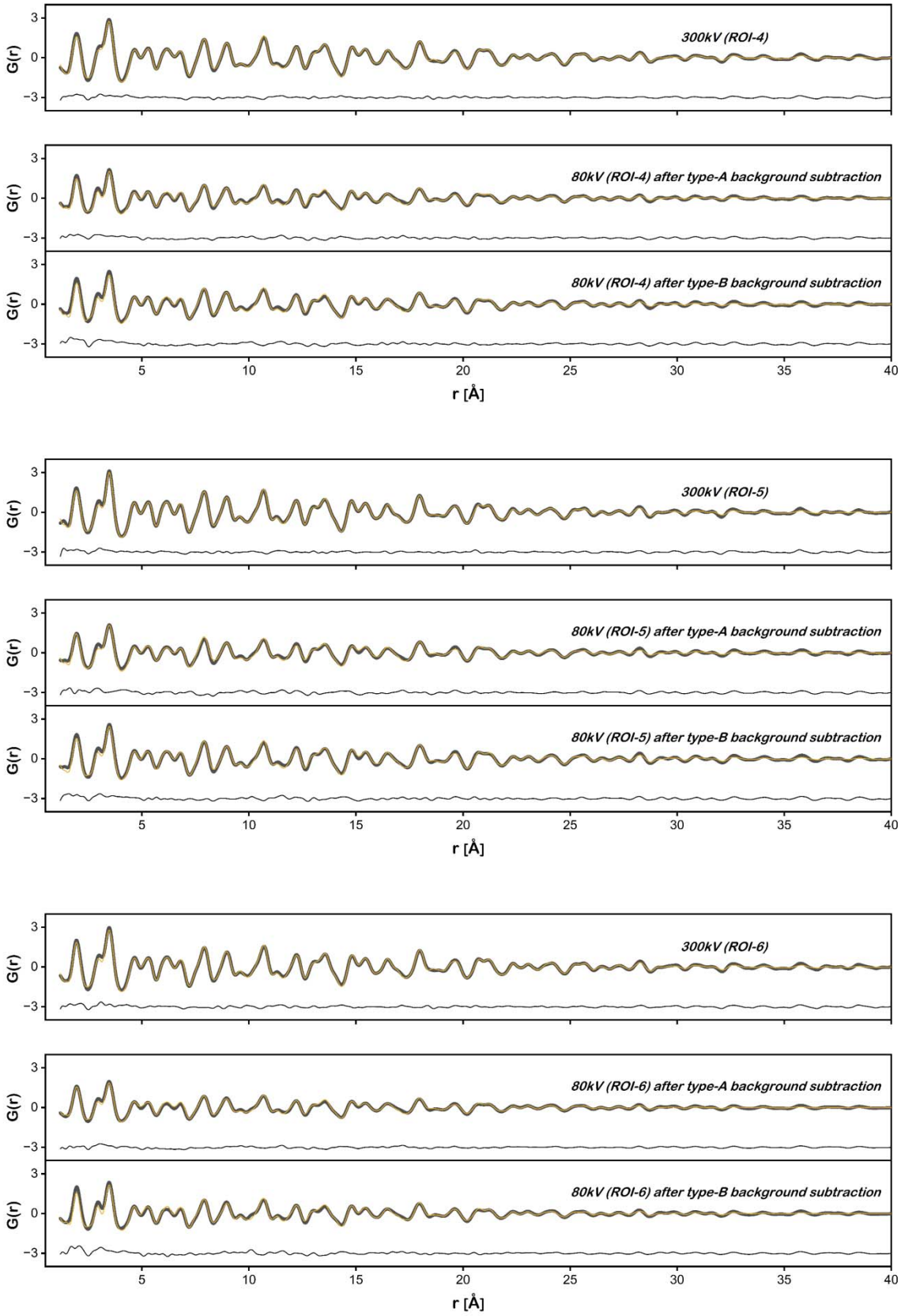

Figure S5 Comparison of refined e-PDF $G(r)$ profiles obtained at various regions of interest (ROI) using 300 kV and 80 kV electron beam energy. Related $\phi(q)$ profiles were overlaid in Fig. 6.

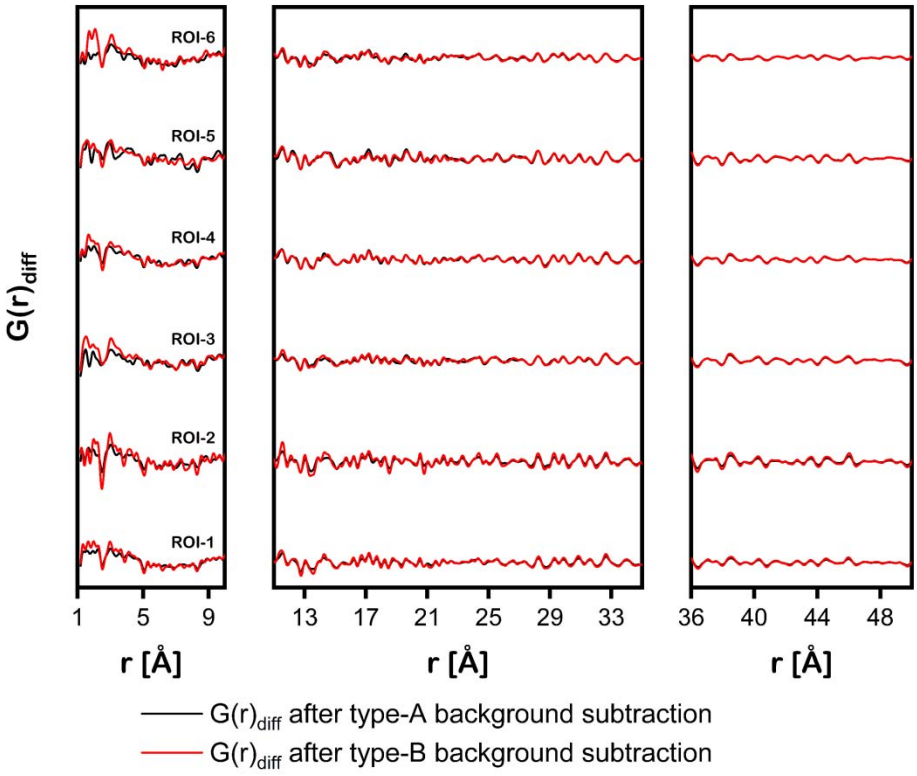

Figure S6 Comparison of $G(r)_{diff}$ of 80 kV e-PDF profiles shown in Fig. S4 and S5. Majority of the difference is found in low-r region (up to 5 Å) between the refined $G(r)$ profiles that have undergone single type-A and double type-B background subtraction. Beyond 5 Å interatomic distance range,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

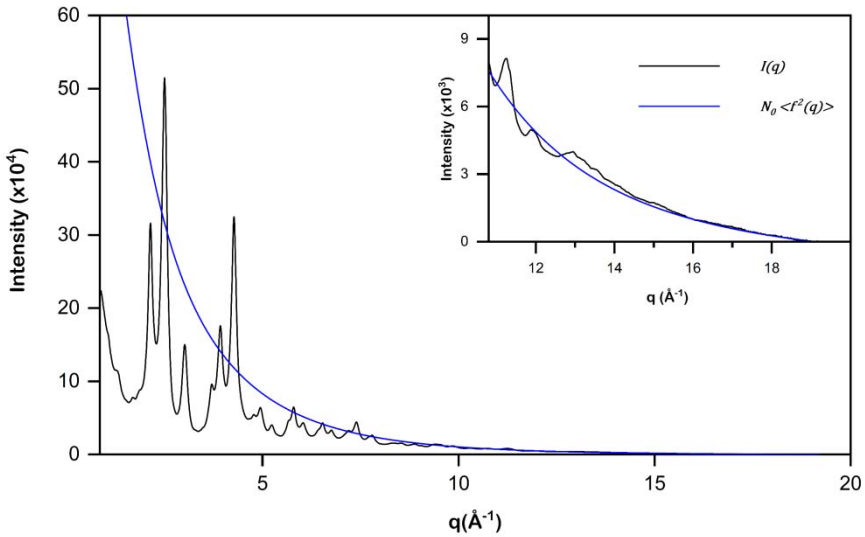

Figure S7 Final $I(q)$ scattering intensity shown in Fig. 5(c) after undergoing type-A followed by type-B background subtraction and mean scattering factor, $N_0\langle f^2(q)\rangle$ fitted at the higher angle (about last one third of the q range).

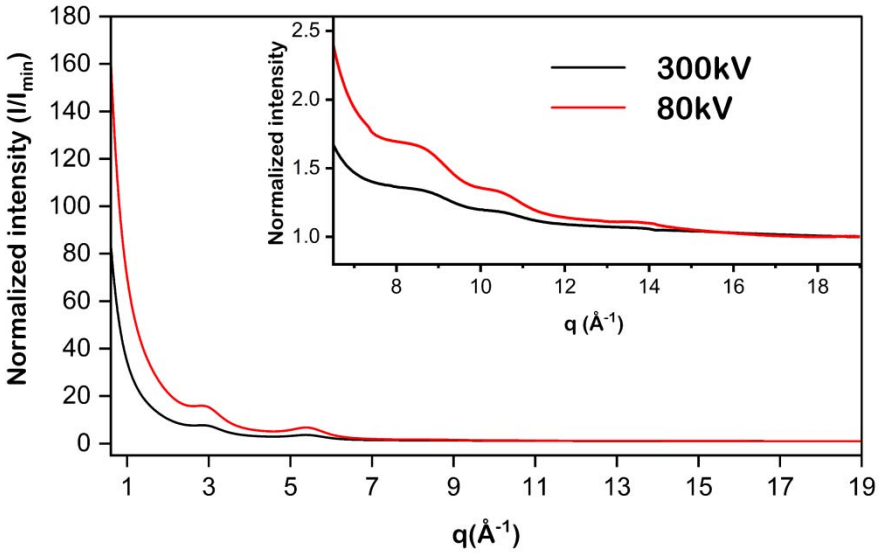

Figure S8 Underneath carbon intensity profiles obtained at 300 kV and 80 kV.

Table S1 Refined parameters of 300 kV e-PDF profiles generated for a damping range of 0 to 0.5 in various Region of interest. Profile with lowest R_w is considered as optimum solution as plotted in Fig. 4.

Region of interest - 1 with damping = 0									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6273	0.8642	0.9786	0.0385	0.0189	0.0011	0.020	1
O2	8b	0.1205	0.3725	0.9987	0.0031	0.0096	0.0001	0.004	1
O3	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***	***y***	***z***	U_{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
O1	8b	0.6208	0.8690	0.9784	0.0131	0.0197	0.0028	0.012	1
O2	8b	0.1175	0.3782	0.9973	0.0207	0.0288	0.0009	0.017	1
O3	8b	0.1289	0.8683	0.0139	0.0206	0.0230	0.0057	0.016	1

O4	8b	0.3664	0.6234	0.9965	0.0147	0.0189	0.0087	0.014	1

Region of interest - 1 with damping = 0.2

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6236	0.8679	0.9806	0.0373	0.0237	0.0052	0.022	1
O2	8b	0.1140	0.3943	1.0020	0.0136	0.0210	0.0190	0.018	1
O3	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 interest - 1 with damping = 0.3

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6175	0.8700	0.9828	0.0241	0.0307	0.0048	0.020	1
O2	8b	0.1257	0.3854	0.9960	0.0422	0.0257	0.0202	0.029	1
O3	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 interest - 1 with damping = 0.4

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6157	0.8722	0.9829	0.0158	0.0381	0.0068	0.020	1
O2	8b	0.1285	0.3825	1.0001	0.0583	0.0291	0.0269	0.038	1
O3	8b	0.1441	0.8749	0.0170	0.0115	0.0229	0.0143	0.016	1
O4	8b	0.3654	0.6198	0.9945	0.0161	0.0179	0.0134	0.016	1

Region of interest - 1 with damping = 0.5

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6116	0.8727	0.9830	0.0132	0.0368	0.0099	0.020	1
O2	8b	0.1343	0.3776	1.0036	0.0488	0.0598	0.0241	0.044	1
O3	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} ($Å^{-1}$)	0.04524	0.03884	0.03921	0.04731	0.04703	0.04752
Q_{broad} ($Å^{-1}$)	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} ***(Å $^{-1}$)*** = 19***; Range (Å)*** = 1.2 – 50***; spdiameter (Å)*** = 52.11(fixed);

Region of interest - 2 with damping = 0									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6190	0.8636	0.9921	0.0318	0.0043	0.0024	0.013	1
O2	8b	0.1219	0.3729	0.9934	0.0109	0.0127	0.0065	0.010	1
O3	8b	0.1320	0.8733	0.0072	0.0171	0.0256	0.0152	0.019	1
O4	8b	0.3743	0.6339	0.9998	0.0194	0.0281	0.0185	0.022	1
Region of interest - 2 with damping = 0.1									
Atom	**Site**	***x***	***y***	***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
O1	8b	0.6123	0.8657	0.9837	0.0103	0.0066	0.0033	0.007	1
O2	8b	0.1158	0.3758	0.9921	0.0089	0.0188	0.0020	0.010	1
O3	8b	0.1296	0.8686	0.0043	0.0143	0.0177	0.0048	0.012	1
O4	8b	0.3697	0.6341	1.0030	0.0131	0.0173	0.0098	0.013	1
Region of interest - 2 with damping = 0.2									
Atom	**Site**	***x***	***y***	***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
O1	8b	0.6139	0.8590	0.9975	0.0665	0.0160	0.0183	0.034	1
O2	8b	0.1126	0.3711	1.0051	0.0188	0.0126	0.0179	0.016	1
O3	8b	0.1271	0.8756	0.0108	0.0327	0.0129	0.0238	0.023	1
O4	8b	0.3960	0.6473	1.0114	0.0188	0.0107	0.0117	0.014	1
Region of interest - 2 with damping = 0.3									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6044	0.8745	0.9807	0.0237	0.0077	0.0203	0.017	1
O2	8b	0.1063	0.3978	0.9900	0.0085	0.0141	0.0096	0.011	1
O3	8b	0.1166	0.8725	0.0007	0.0003	0.0232	0.0144	0.013	1
O4	8b	0.3746	0.6276	0.9789	0.0257	0.0179	0.0082	0.017	1
Region of interest - 2 with damping = 0.4									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6434	0.8708	0.9919	0.0091	0.0397	0.0087	0.019	1
O2	8b	0.1192	0.3778	1.0029	0.0090	0.0202	0.0290	0.019	1
O3	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

Region of interest - 2 with damping = 0.5									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6185	0.8641	0.9736	0.0089	0.0234	0.0197	0.017	1
O2	8b	0.1257	0.3910	0.9949	0.0658	0.0219	0.0555	0.048	1
O3	8b	0.1452	0.8702	0.0098	0.0198	0.0397	0.0310	0.030	1
O4	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} ($Å^{-1}$)	0.04196	0.03945	0.04467	0.04240	0.04160	0.04304
Q_{broad} ($Å^{-1}$)	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

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

Region of interest - 3 with damping = 0									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6183	0.8616	0.9942	0.0229	0.0188	0.0224	0.021	1
O2	8b	0.1242	0.3724	0.9933	0.0089	0.0083	0.0103	0.009	1
O3	8b	0.1328	0.8709	0.0083	0.0121	0.0176	0.0139	0.015	1
O4	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***	***y***	***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
O1	8b	0.6232	0.8748	0.9858	0.0325	0.0282	0.0144	0.025	1
O2	8b	0.1082	0.3649	1.0027	0.0121	0.0216	0.0140	0.016	1
O3	8b	0.1317	0.8784	0.0050	0.0133	0.0260	0.0071	0.015	1
O4	8b	0.3710	0.6312	1.0035	0.0126	0.0146	0.0182	0.015	1

Region of interest - 3 with damping = 0.2

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6139	0.8750	0.9806	0.0277	0.0313	0.0041	0.021	1
O2	8b	0.1131	0.3804	0.9746	0.0625	0.0031	0.0423	0.036	1
O3	8b	0.1313	0.8636	0.0043	0.0279	0.0268	0.0122	0.022	1
O4	8b	0.3696	0.6236	0.9915	0.0104	0.0084	0.0021	0.007	1

Region of interest - 3 with damping = 0.3

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6216	0.8755	0.9921	0.0112	0.0301	0.0081	0.016	1
O2	8b	0.1162	0.3641	0.9642	0.0269	0.0572	0.0894	0.058	1
O3	8b	0.1166	0.8723	0.0105	0.0107	0.0284	0.0120	0.017	1
O4	8b	0.3595	0.6321	0.9771	0.0129	0.0235	0.0061	0.014	1

Region of interest - 3 with damping = 0.4

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6218	0.8652	0.9888	0.0220	0.0383	0.0202	0.027	1
O2	8b	0.1230	0.3872	0.9901	0.0489	0.0231	0.0674	0.046	1
O3	8b	0.1420	0.8805	0.0057	0.0159	0.0683	0.0259	0.037	1
O4	8b	0.3724	0.6234	0.9899	0.0140	0.0251	0.0116	0.017	1

Region of interest - 3 with damping = 0.5

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6273	0.8770	0.9918	0.0209	0.0217	0.0190	0.021	1
O2	8b	0.1156	0.3634	0.9676	0.0517	0.0445	0.0913	0.062	1
O3	8b	0.1204	0.8743	0.0070	0.0214	0.0402	0.0143	0.025	1
O4	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} ($Å^{-1}$)	0.05028	0.04856	0.04796	0.04779	0.04994	0.04983
Q_{broad} ($Å^{-1}$)	0.00206	0.00998	0.00175	0.00121	0.00124	0.00336

R_w (%)	20.58	12.13	12.43	11.20	11.67	12.32

Q_{max} (Å^{-1}) = 19; **Range (Å)** = 1.2 – 50; **spdiameter (Å)** = 52.11(fixed);

Region of interest - 4 with damping = 0

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6150	0.8675	0.9844	0.0475	0.0033	0.0023	0.018	1
O2	8b	0.1232	0.3756	0.9885	0.0309	0.0223	0.0033	0.019	1
O3	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 interest - 4 with damping = 0.1

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6120	0.8682	0.9845	0.0015	0.0490	0.0040	0.018	1
O2	8b	0.1179	0.3799	0.9905	0.0168	0.0306	0.0139	0.020	1
O3	8b	0.1318	0.8777	0.0061	0.0410	0.0111	0.0077	0.020	1
O4	8b	0.3727	0.6313	1.0064	0.0018	0.0085	0.0041	0.005	1

Region of interest - 4 with damping = 0.2

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6165	0.8695	0.9799	0.0125	0.0412	0.0045	0.019	1
O2	8b	0.0979	0.3993	1.0036	0.0219	0.0238	0.0030	0.016	1
O3	8b	0.1486	0.8715	0.0119	0.0346	0.0093	0.0065	0.017	1
O4	8b	0.3821	0.6141	0.9944	0.0060	0.0055	0.0045	0.005	1

Region of interest - 4 with damping = 0.3

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6164	0.8778	0.9788	0.0122	0.0315	0.0133	0.019	1
O2	8b	0.1205	0.3850	0.9827	0.0376	0.0174	0.0230	0.026	1
O3	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 damping = 0.4

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6308	0.8702	0.9646	0.0756	0.0091	0.0180	0.034	1
O2	8b	0.1167	0.3852	0.9998	0.0093	0.0109	0.0144	0.012	1
O3	8b	0.1531	0.8687	0.0255	0.0704	0.0126	0.0079	0.030	1
O4	8b	0.3898	0.6114	0.9947	0.0103	0.0110	0.0154	0.012	1

Region of interest - 4 with damping = 0.5									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6381	0.8799	0.9676	0.0438	0.0194	0.0117	0.025	1
O2	8b	0.1233	0.3793	1.0014	0.0208	0.0168	0.0182	0.019	1
O3	8b	0.1673	0.8731	0.0282	0.1094	0.0150	0.0144	0.046	1
O4	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} ($Å^{-1}$)	0.04911	0.04556	0.04539	0.04214	0.04394	0.04506
Q_{broad} ($Å^{-1}$)	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

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

Region of interest - 5 with damping = 0									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6183	0.8652	0.9938	0.0218	0.0021	0.0018	0.009	1
O2	8b	0.1224	0.3729	0.9919	0.0141	0.0112	0.0021	0.009	1
O3	8b	0.1301	0.8732	0.0061	0.0105	0.0205	0.0046	0.012	1
O4	8b	0.3749	0.6329	0.9996	0.0144	0.0143	0.0025	0.010	1
Region of interest - 5 with damping = 0.1									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6144	0.8655	0.9920	0.0057	0.0137	0.0243	0.015	1
O2	8b	0.1179	0.3749	0.9885	0.0172	0.0179	0.0083	0.014	1
O3	8b	0.1285	0.8702	0.0061	0.0158	0.0184	0.0052	0.013	1
O4	8b	0.3744	0.6323	1.0017	0.0107	0.0306	0.0108	0.017	1
Region of interest - 5 with damping = 0.2									
Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6054	0.8695	0.9952	0.0229	0.0054	0.0184	0.016	1
O2	8b	0.1101	0.3919	0.9852	0.0246	0.0152	0.0129	0.018	1
O3	8b	0.1350	0.8765	0.0068	0.0172	0.0220	0.0073	0.016	1
O4	8b	0.3655	0.6242	0.9989	0.0124	0.0080	0.0088	0.010	1

Region of interest - 5 with damping = 0.3

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6262	0.8673	0.9833	0.0259	0.0145	0.0346	0.025	1
O2	8b	0.0997	0.3844	0.9832	0.0051	0.0150	0.0133	0.011	1
O3	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 interest - 5 with damping = 0.4

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6200	0.8694	0.9829	0.0120	0.0262	0.0120	0.017	1
O2	8b	0.1291	0.3906	0.9875	0.0519	0.0024	0.0224	0.026	1
O3	8b	0.1413	0.8751	0.0161	0.0235	0.0090	0.0211	0.018	1
O4	8b	0.3716	0.6219	0.9935	0.0142	0.0321	0.0060	0.017	1

Region of interest - 5 with damping = 0.5

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6300	0.8661	0.9913	0.0167	0.0483	0.0397	0.035	1
O2	8b	0.1172	0.3831	0.9978	0.0131	0.0137	0.0173	0.015	1
O3	8b	0.1369	0.8662	0.0243	0.0203	0.0199	0.0061	0.015	1
O4	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} ($Å^{-1}$)	0.04657	0.04565	0.04565	0.04771	0.05026	0.05014
Q_{broad} ($Å^{-1}$)	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} ($Å^{-1}$) = 19***; Range (Å)*** = 1.2 – 50***; spdiameter (Å)*** = 52.11(fixed);

Region of interest - 6 with damping = 0

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6187	0.8624	0.9887	0.0197	0.0025	0.0042	0.009	1
O2	8b	0.1196	0.3711	0.9946	0.0061	0.0132	0.0067	0.009	1
O3	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 interest - 6 with damping = 0.1

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6125	0.8672	0.9879	0.0069	0.0073	0.0114	0.009	1
O2	8b	0.1139	0.3811	0.9929	0.0116	0.0224	0.0073	0.014	1
O3	8b	0.1367	0.8780	0.0062	0.0269	0.0169	0.0112	0.018	1
O4	8b	0.3726	0.6323	1.0051	0.0063	0.0184	0.0104	0.012	1

Region of interest - 6 with damping = 0.2

Atom	**Site**	***x***	***y***	***z***	U_{11}	U_{22}	U_{33}	U_{iso}	**S.O.F.**
Fe1	8b	0.7417	0.9980	0.1127	0.0065	0.0083	0.0258	0.014	0.699
Fe2	4a	0.6329	0.6329		0.0108	0.0108	0.0062	0.009	0.605
Fe3	8b	0.3682	0.8723	0.9795	0.0100	0.0127	0.0144	0.012	0.538
Fe4	4a	0.1262	0.1262		0.0032	0.0032	0.0122	0.006	0.333
O1	8b	0.6224	0.8826	0.9755	0.0163	0.0457	0.0035	0.022	1
O2	8b	0.1120	0.3969	1.0003	0.0365	0.0072	0.0116	0.018	1
O3	8b	0.1412	0.8842	0.0177	0.0524	0.0019	0.0072	0.020	1
O4	8b	0.3722	0.6313	1.0001	0.0104	0.0050	0.0085	0.008	1

Region of interest - 6 with damping = 0.3

Atom	**Site**	***x***	***y***	***z***	U_{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
O1	8b	0.6420	0.8821	0.9719	0.0222	0.0278	0.0043	0.018	1
O2	8b	0.1217	0.3777	0.9979	0.0217	0.0161	0.0166	0.018	1
O3	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

Region of interest - 6 with damping = 0.4

Atom	**Site**	***x***	***y***	***z***	U_{11}	U_{22}	U_{33}	U_{iso}	**S.O.F.**
Fe1	8b	0.7458	0.9984	0.1112	0.0164	0.0103	0.0383	0.022	0.655
Fe2	4a	0.6361	0.6361		0.0163	0.0163	0.0226	0.018	0.613
Fe3	8b	0.3676	0.8713	0.9892	0.0126	0.0168	0.0062	0.012	0.320
Fe4	4a	0.1224	0.1224		0.0112	0.0112	0.0154	0.013	0.333
O1	8b	0.6418	0.8816	0.9723	0.0210	0.0307	0.0046	0.019	1
O2	8b	0.1206	0.3777	0.9991	0.0231	0.0147	0.0156	0.018	1
O3	8b	0.1513	0.8750	0.0276	0.0150	0.0211	0.0103	0.015	1
O4	8b	0.3838	0.6229	0.9919	0.0116	0.0290	0.0170	0.019	1

Region of interest - 6 with damping = 0.5

Atom	**Site**	***x***	***y***	***z***	U_{11}	U_{22}	U_{33}	U_{iso}	**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
O1	8b	0.6412	0.8827	0.9727	0.0376	0.0313	0.0043	0.024	1
O2	8b	0.1209	0.3793	0.9986	0.0226	0.0184	0.0156	0.019	1
O3	8b	0.1524	0.8757	0.0282	0.0194	0.0132	0.0155	0.016	1
O4	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} (Å^{-1})	0.04493	0.04641	0.04654	0.04642	0.04827	0.04655
Q_{broad} (Å^{-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} (Å^{-1}) = 19; **Range (Å)** = 1.2 – 50; **spdiameter (Å)** = 52.11(fixed);

Table S2 Refined parameters related to the profiles shown in Fig. S4 and S5

300 kV (ROI-1)

Q_{max} (Å^{-1}) = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.693; **a (Å)** = 8.3446; **c (Å)** = 8.2858; **damping** = 0.2; δ_2 = 3.12; Q_{damp} (Å^{-1}) = 0.03921; Q_{broad} (Å^{-1}) = 0.00383; **spdiameter (Å)** = 52.11 (fixed); R_w (%) = 10.51

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6236	0.8679	0.9806	0.0373	0.0237	0.0052	0.022	1
O2	8b	0.1140	0.3943	1.0020	0.0136	0.0210	0.0190	0.018	1
O3	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

80 kV (ROI-1) after type-A background subtraction

Q_{max} (Å^{-1}) = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.577; **a (Å)** = 8.3567; **c (Å)** = 8.2795; **damping** = 0.4; δ_2 = 3.05; Q_{damp} (Å^{-1}) = 0.05124; Q_{broad} (Å^{-1}) = 0.00242; **spdiameter (Å)** = 52.11 (fixed); R_w (%) = 20.47

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{iso}	S.O.F.
Fe1	8b	0.7401	0.9973	0.1159	0.0091	0.0176	0.0299	0.019	0.633
Fe2	4a	0.6369	0.6369		0.0037	0.0037	0.0000	0.002	0.222
Fe3	8b	0.3713	0.8685	0.9925	0.0206	0.0124	0.0191	0.017	0.523
Fe4	4a	0.1244	0.1244		0.0096	0.0096	0.0158	0.012	0.333
O1	8b	0.6112	0.8733	0.9886	**0.2206**	**0.1421**	**0.0314**	0.131	1
O2	8b	0.1271	0.3839	0.9998	0.0259	0.0123	0.0529	0.030	1
O3	8b	0.1253	0.8802	0.0109	0.0618	0.0170	0.0284	0.036	1
O4	8b	0.3764	0.6319	0.9947	0.0486	0.0023	0.0214	0.024	1

80 kV (ROI-1) after type- background subtraction

Q_{max} (Å^{-1}) = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.689; **a (Å)** = 8.3534; **c (Å)** = 8.2871; **damping** = 0.3; δ_2 = 3.09; Q_{damp} (Å^{-1}) = 0.05054; Q_{broad} (Å^{-1}) = 0.00457; **spdiameter (Å)** = 52.11 (fixed); R_w (%) = 21.06

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{iso}	S.O.F.
Fe1	8b	0.7375	0.9934	0.1159	0.0070	0.0150	0.0139	0.012	0.647
Fe2	4a	0.6293	0.6293		0.0125	0.0125	0.0058	0.010	0.261
Fe3	8b	0.3677	0.8655	0.9969	0.0169	0.0070	0.0192	0.014	0.522

Fe4	4a	0.1291	0.1291		0.0060	0.0060	0.0099	0.007	0.333
O1	8b	0.6149	0.8813	0.9856	0.0654	0.0293	0.0951	0.063	1
O2	8b	0.1108	0.3714	0.9832	0.0152	0.0170	0.0358	0.023	1
O3	8b	0.1259	0.8640	0.0157	0.0093	0.0131	0.0184	0.014	1
O4	8b	0.3718	0.6139	0.9876	0.0311	0.0129	0.0113	0.018	1

300 kV (ROI-2)

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.759; **a (Å)** = 8.3540; **c (Å)** = 8.2885; **damping** = 0.4; **δ_2** = 2.49; **Q_{damp} (Å^{-1})** = 0.04160; **Q_{broad} (Å^{-1})** = 0.00047; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 11.36*

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6434	0.8708	0.9919	0.0091	0.0397	0.0087	0.019	1
O2	8b	0.1192	0.3778	1.0029	0.0090	0.0202	0.0290	0.019	1
O3	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-A background subtraction

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.662; **a (Å)** = 8.3499; **c (Å)** = 8.3009; **damping** = 0.4; **δ_2** = 3.16; **Q_{damp} (Å^{-1})** = 0.04728; **Q_{broad} (Å^{-1})** = 0.00087; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 19.16*

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{iso}	S.O.F.
Fe1	8b	0.7426	0.9992	0.1130	0.0143	0.0137	0.0251	0.018	0.597
Fe2	4a	0.6377	0.6377		0.0111	0.0111	0.0160	0.013	0.450
Fe3	8b	0.3676	0.8721	0.9887	0.0139	0.0124	0.0082	0.012	0.439
Fe4	4a	0.1247	0.1247		0.0100	0.0100	0.0171	0.012	0.333
O1	8b	0.6102	0.8681	0.9913	0.0601	0.0519	0.0097	0.041	1
O2	8b	0.1262	0.3835	1.0009	0.0259	0.0177	0.0049	0.016	1
O3	8b	0.1502	0.8830	0.0153	**0.4744**	**0.1128**	**0.0830**	0.223	1
O4	8b	0.3807	0.6361	1.0019	0.0298	0.0017	0.0421	0.025	1

80 kV (ROI-2) after type- background subtraction

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.730; **a (Å)** = 8.3566; **c (Å)** = 8.2828; **damping** = 0.3; **δ_2** = 3.21; **Q_{damp} (Å^{-1})** = 0.04482; **Q_{broad} (Å^{-1})** = 0.00909; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 19.16*

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{iso}	S.O.F.
Fe1	8b	0.7393	0.9959	0.1114	0.0110	0.0086	0.0133	0.011	0.737
Fe2	4a	0.6382	0.6382		0.0108	0.0108	0.0071	0.010	0.547
Fe3	8b	0.3659	0.8748	0.9870	0.0090	0.0120	0.0103	0.010	0.717
Fe4	4a	0.1264	0.1264		0.0050	0.0050	0.0053	0.005	0.333
O1	8b	0.6087	0.8731	0.9901	0.0121	0.0275	0.0178	0.019	1
O2	8b	0.1212	0.3949	0.9958	0.0205	0.0138	0.0020	0.012	1
O3	8b	0.1293	0.8862	0.0105	0.0255	0.0299	0.0197	0.025	1
O4	8b	0.3822	0.6379	1.0013	0.0130	0.0002	0.0181	0.010	1

300 kV (ROI-3)

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.749; **a (Å)** = 8.3404; **c (Å)** = 8.3005; **damping** = 0.3; **δ_2** = 2.88; **Q_{damp} (Å^{-1})** = 0.04779; **Q_{broad} (Å^{-1})** = 0.00121; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 11.20*

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6216	0.8755	0.9921	0.0112	0.0301	0.0081	0.016	1
O2	8b	0.1162	0.3641	0.9642	0.0269	0.0572	0.0894	0.058	1
O3	8b	0.1166	0.8723	0.0105	0.0107	0.0284	0.0120	0.017	1
O4	8b	0.3595	0.6321	0.9771	0.0129	0.0235	0.0061	0.014	1

80 kV (ROI-3) after type-A background subtraction

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.728; **a (Å)** = 8.3576; **c (Å)** = 8.2640; **damping** = 0.4; **δ_2** = 2.92; **Q_{damp} (Å^{-1})** = 0.04601; **Q_{broad} (Å^{-1})** = 0.00882; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 16.74*

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{iso}	S.O.F.
Fe1	8b	0.7561	1.0029	0.1242	0.0137	0.0251	0.0332	0.024	0.543
Fe2	4a	0.6385	0.6385		0.0093	0.0093	0.0087	0.009	0.353
Fe3	8b	0.3687	0.8680	0.9875	0.0073	0.0076	0.0054	0.007	0.284
Fe4	4a	0.1255	0.1255		0.0145	0.0145	0.0104	0.013	0.333
O1	8b	0.6065	0.8432	0.9891	**0.0278**	**3.5994**	**0.0236**	1.217	1
O2	8b	0.1289	0.3851	1.0078	0.0281	0.0235	0.0310	0.028	1
O3	8b	0.1368	0.8692	0.0225	0.0093	0.0458	0.0297	0.028	1
O4	8b	0.3835	0.6265	0.9896	0.0288	0.0126	0.0253	0.022	1

80 kV (ROI-3) after type- background subtraction

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.691; **a (Å)** = 8.3518; **c (Å)** = 8.2706; **damping** = 0.4; **δ_2** = 2.80; **Q_{damp} (Å^{-1})** = 0.04515; **Q_{broad} (Å^{-1})** = 0.00106; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 19.63*

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{iso}	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		0.0137	0.0137	0.0079	0.012	0.333
O1	8b	0.6269	0.8490	0.9803	0.0287	0.0563	0.0010	0.029	1
O2	8b	0.1169	0.3913	1.0076	0.0180	0.0080	0.0146	0.014	1
O3	8b	0.1193	0.8695	0.0094	0.0464	0.0369	0.0362	0.040	1
O4	8b	0.3818	0.6333	0.9867	0.0306	0.0035	0.0127	0.016	1

300 kV (ROI-4)

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.845; **a (Å)** = 8.3480; **c (Å)** = 8.2979; **damping** = 0.4; **δ_2** = 2.95; **Q_{damp} (Å^{-1})** = 0.04394; **Q_{broad} (Å^{-1})** = 0.00118; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 11.70*

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6308	0.8702	0.9646	0.0756	0.0091	0.0180	0.034	1
O2	8b	0.1167	0.3852	0.9998	0.0093	0.0109	0.0144	0.012	1
O3	8b	0.1531	0.8687	0.0255	0.0704	0.0126	0.0079	0.030	1
O4	8b	0.3898	0.6114	0.9947	0.0103	0.0110	0.0154	0.012	1

80 kV (ROI-4) after type-A background subtraction

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.587; **a (Å)** = 8.3519; **c (Å)** = 8.2775; **damping** = 0.3; **δ_2** = 3.20; **Q_{damp} (Å^{-1})** = 0.05156; **Q_{broad} (Å^{-1})** = 0.00044; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 20.36*

Atom	Site	*x*	*y*	*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
O1	8b	0.5989	0.8755	0.9681	**0.3188**	**0.1068**	**0.1948**	0.207	1
O2	8b	0.1125	0.3755	0.9778	0.0078	0.0277	0.0302	0.022	1
O3	8b	0.1297	0.8644	0.0104	0.0273	0.0255	0.0155	0.023	1
O4	8b	0.3787	0.6179	0.9906	0.0205	0.0094	0.0104	0.013	1

80 kV (ROI-4) after type- background subtraction

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.610; **a (Å)** = 8.3560; **c (Å)** = 8.2734; **damping** = 0.4; **δ_2** = 3.17; **Q_{damp} (Å^{-1})** = 0.05193; **Q_{broad} (Å^{-1})** = 0.00307; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 22.07*

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6225	0.8687	0.9908	0.0330	0.0112	0.0166	0.020	1
O2	8b	0.1149	0.3823	0.9907	0.0215	0.0424	0.0673	0.044	1
O3	8b	0.1363	0.8772	0.0064	0.0751	0.0379	0.0155	0.043	1
O4	8b	0.3737	0.6272	0.9908	0.0329	0.0170	0.0428	0.031	1

300 kV (ROI-5)

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.726; **a (Å)** = 8.3433; **c (Å)** = 8.2986; **damping** = 0.3; **δ_2** = 3.04; **Q_{damp} (Å^{-1})** = 0.04771; **Q_{broad} (Å^{-1})** = 0.00426; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 11.71*

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6262	0.8673	0.9833	0.0259	0.0145	0.0346	0.025	1
O2	8b	0.0997	0.3844	0.9832	0.0051	0.0150	0.0133	0.011	1
O3	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

80 kV (ROI-5) after type-A background subtraction

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.568; **a (Å)** = 8.3578; **c (Å)** = 8.2845; **damping** = 0.4; **δ_2** = 3.17; **Q_{damp} (Å^{-1})** = 0.04763; **Q_{broad} (Å^{-1})** = 0.00676; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 22.31*

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{iso}	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
O1	8b	0.6178	0.8524	0.9963	**0.0239**	**0.1658**	**0.0125**	0.067	1
O2	8b	0.1179	0.3962	0.9974	0.0142	0.0151	0.0276	0.019	1
O3	8b	0.1199	0.8869	0.0168	0.0798	0.0000	0.0110	0.030	1
O4	8b	0.3668	0.6267	0.9890	0.0073	0.0084	0.0237	0.013	1

80 kV (ROI-5) after type- background subtraction

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.672; **a (Å)** = 8.3554; **c (Å)** = 8.2885; **damping** = 0.4; **δ_2** = 3.01; **Q_{damp} (Å^{-1})** = 0.04589; **Q_{broad} (Å^{-1})** = 0.00029; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 18.93*

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{iso}	S.O.F.
Fe1	8b	0.7399	1.0021	0.1124	0.0081	0.0133	0.0291	0.017	0.689
Fe2	4a	0.6332	0.6332		0.0161	0.0161	0.0244	0.019	0.677
Fe3	8b	0.3684	0.8712	0.9899	0.0127	0.0097	0.0043	0.009	0.377
Fe4	4a	0.1280	0.1280		0.0108	0.0108	0.0066	0.009	0.333
O1	8b	0.6215	0.8650	0.9891	0.0316	0.0155	0.0215	0.023	1
O2	8b	0.1225	0.3864	1.0013	0.0292	0.0164	0.0066	0.017	1
O3	8b	0.1366	0.8842	0.0197	0.0522	0.0844	0.0442	0.060	1
O4	8b	0.3764	0.6350	0.9952	0.0414	0.0168	0.0315	0.030	1

300 kV (ROI-6)

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.794; **a (Å)** = 8.3451; **c (Å)** = 8.2988; **damping** = 0.3; **δ_2** = 2.83; **Q_{damp} (Å^{-1})** = 0.04642; **Q_{broad} (Å^{-1})** = 0.00290; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 13.05*

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6420	0.8821	0.9719	0.0222	0.0278	0.0043	0.018	1
O2	8b	0.1217	0.3777	0.9979	0.0217	0.0161	0.0166	0.018	1
O3	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} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.647; **a (Å)** = 8.3489; **c (Å)** = 8.2741; **damping** = 0.4; **δ_2** = 3.21; **Q_{damp} (Å^{-1})** = 0.05272; **Q_{broad} (Å^{-1})** = 0.00421; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 18.50*

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.5642	0.9484	0.9420	**0.1559**	**4.8663**	**0.0955**	1.706	1
O2	8b	0.1092	0.3763	0.9807	0.0054	0.0241	0.0563	0.029	1
O3	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-6) after type- background subtraction

***Q_{max} (Å^{-1})** = 19; **Range (Å)** = 1.2 – 50; **scale factor** = 0.511; **a (Å)** = 8.3583; **c (Å)** = 8.2664; **damping** = 0.3; **δ_2** = 3.07; **Q_{damp} (Å^{-1})** = 0.05171; **Q_{broad} (Å^{-1})** = 0.00572; **spdiameter (Å)** = 52.11 (fixed); **R_w (%)** = 25.06*

Atom	Site	*x*	*y*	*z*	U_{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
O1	8b	0.6158	0.8642	0.9887	0.0031	0.0141	0.0233	0.014	1
O2	8b	0.1170	0.3843	1.0000	0.0100	0.0221	0.0075	0.013	1
O3	8b	0.1434	0.8731	0.0153	0.0120	0.0345	0.0890	0.045	1
O4	8b	0.3762	0.6277	0.9944	0.0198	0.0621	0.0112	0.031	1

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