Supporting Online Material for

Neutron Pair Distribution Function Study of 2-line Ferrihydrite

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Figure S1. Thermogravimetric analysis (TGA) of 2-line ferrihydrite heated under vacuum.
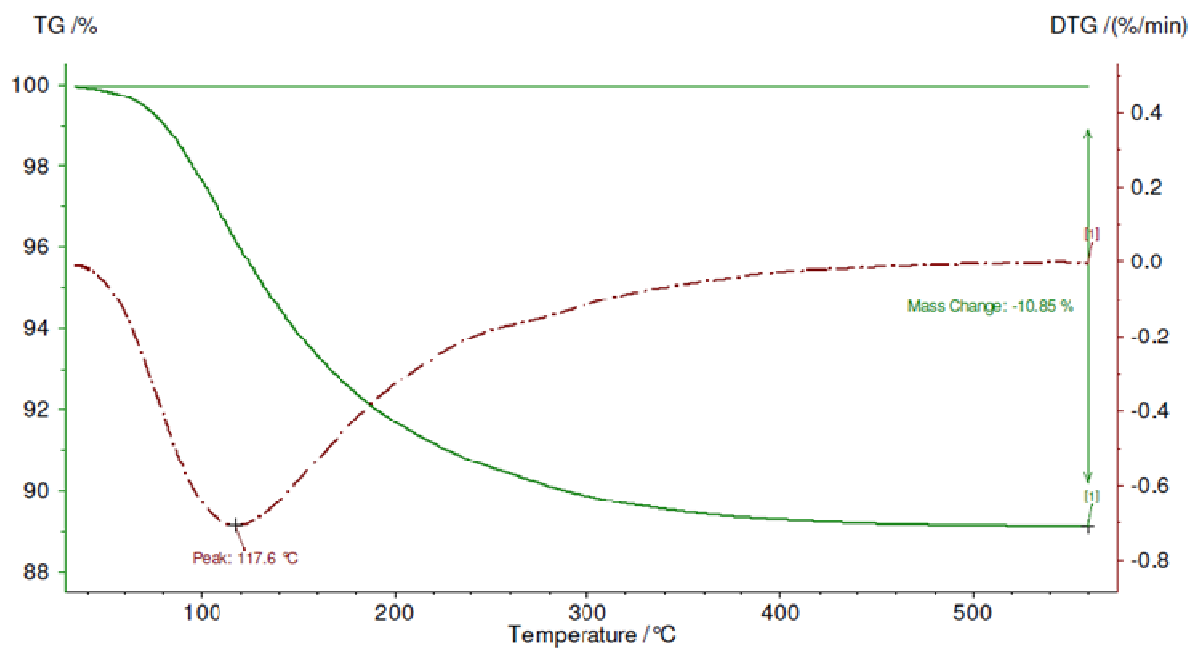
Fits to other iron oxides and oxyhydroxides.

Figure S2. Fit of the hematite structure to the neutron PDF data. The blue circles are the experimental data, the red line the calculated curve and the green curve the difference between them. Rw = 79%.
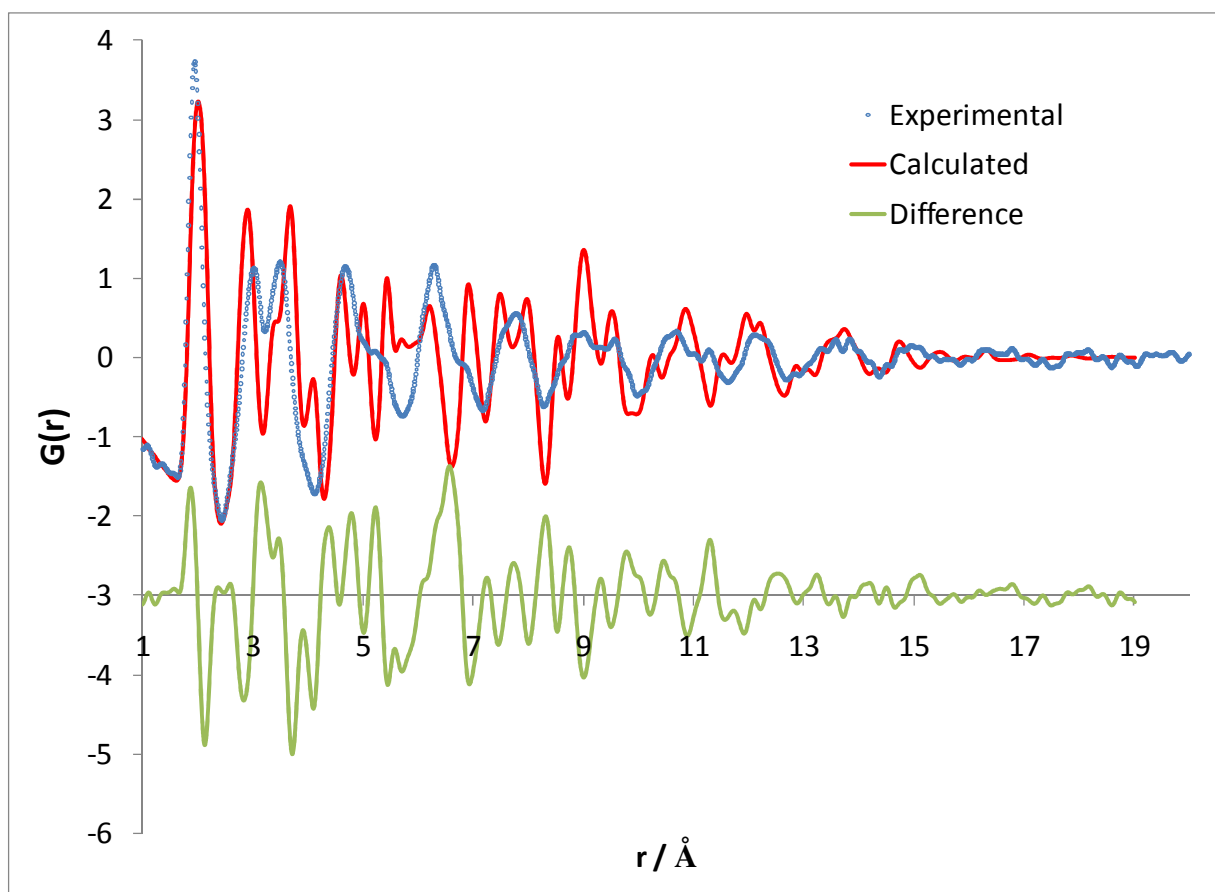
**Figure S3, Magnetite,** Fe_3O_4

Refined the scale factor and Sratio. The positions of the peaks are reasonable, but the intensities are mismatched, especially at low r where it would be expected the fit would be the best. The 3rd peak is large as it contains contributions from Fe-O and Fe-Fe correlations.
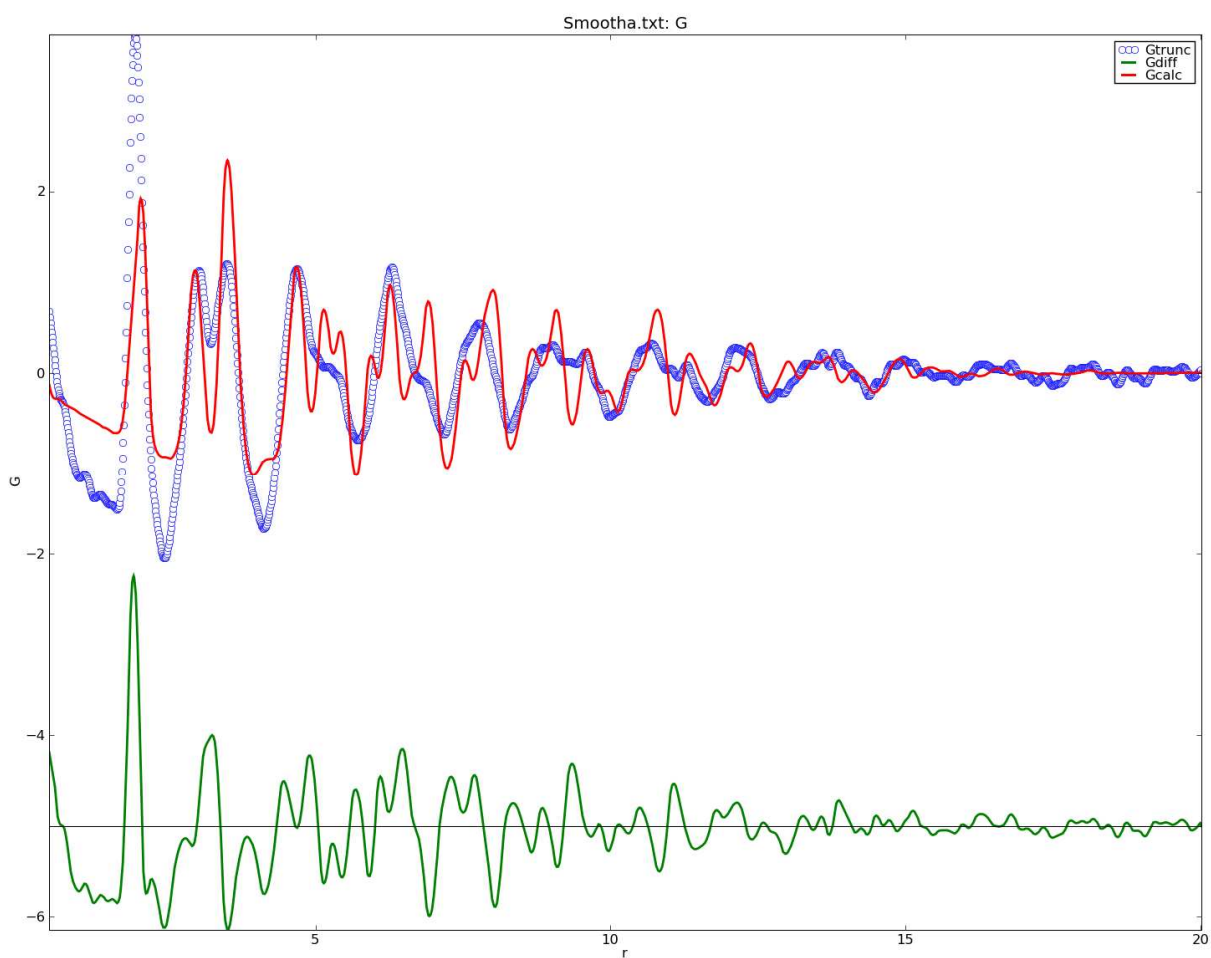
Figure S4, Maghemite, $Fe_{2.677}O_4$

Refined scale, sratio, U_{Fe} and U_O (as the CIF gives no Uiso values). The fit is reasonably good. The fit to the first peak is poor, it appears to be 2 separate peaks.
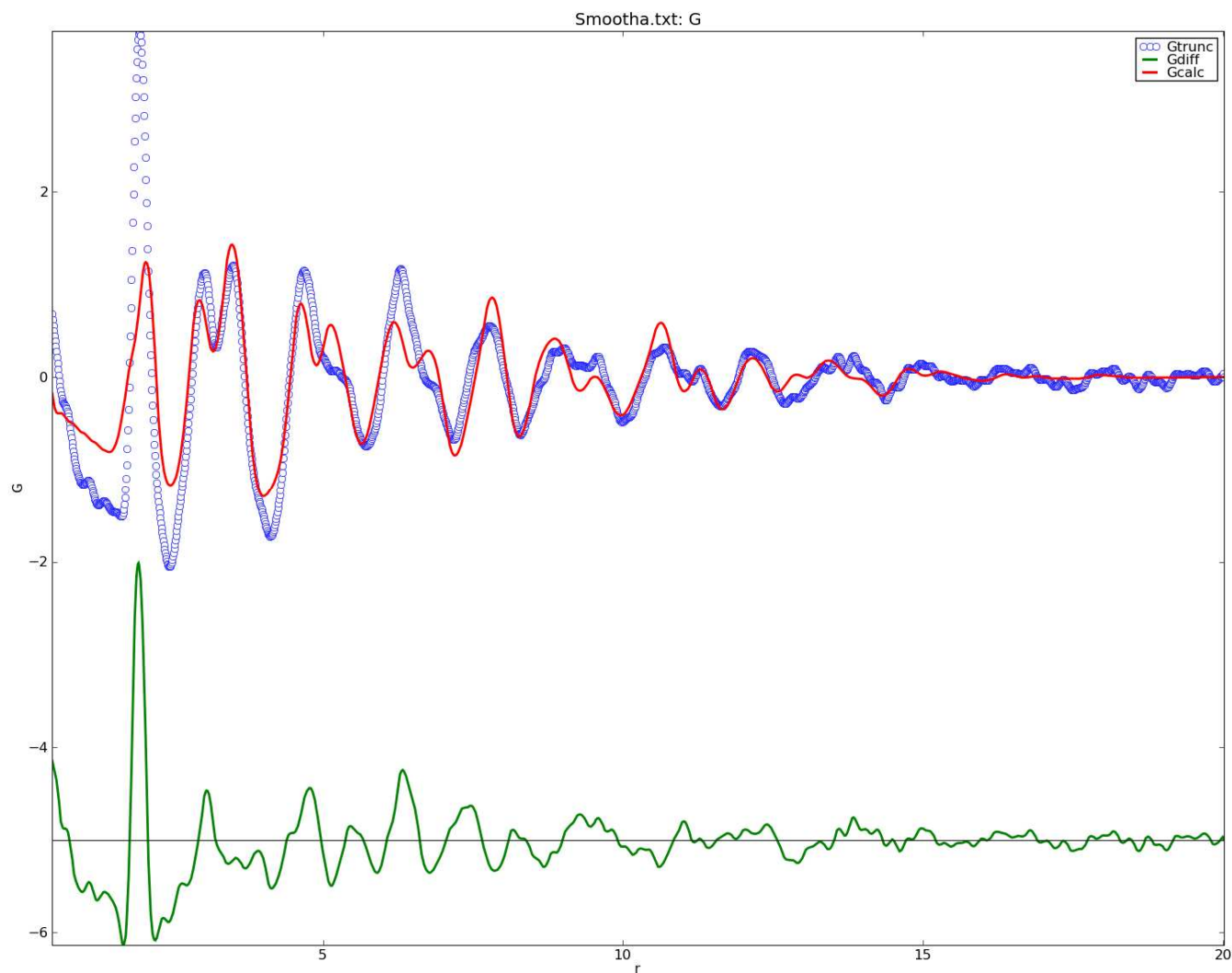
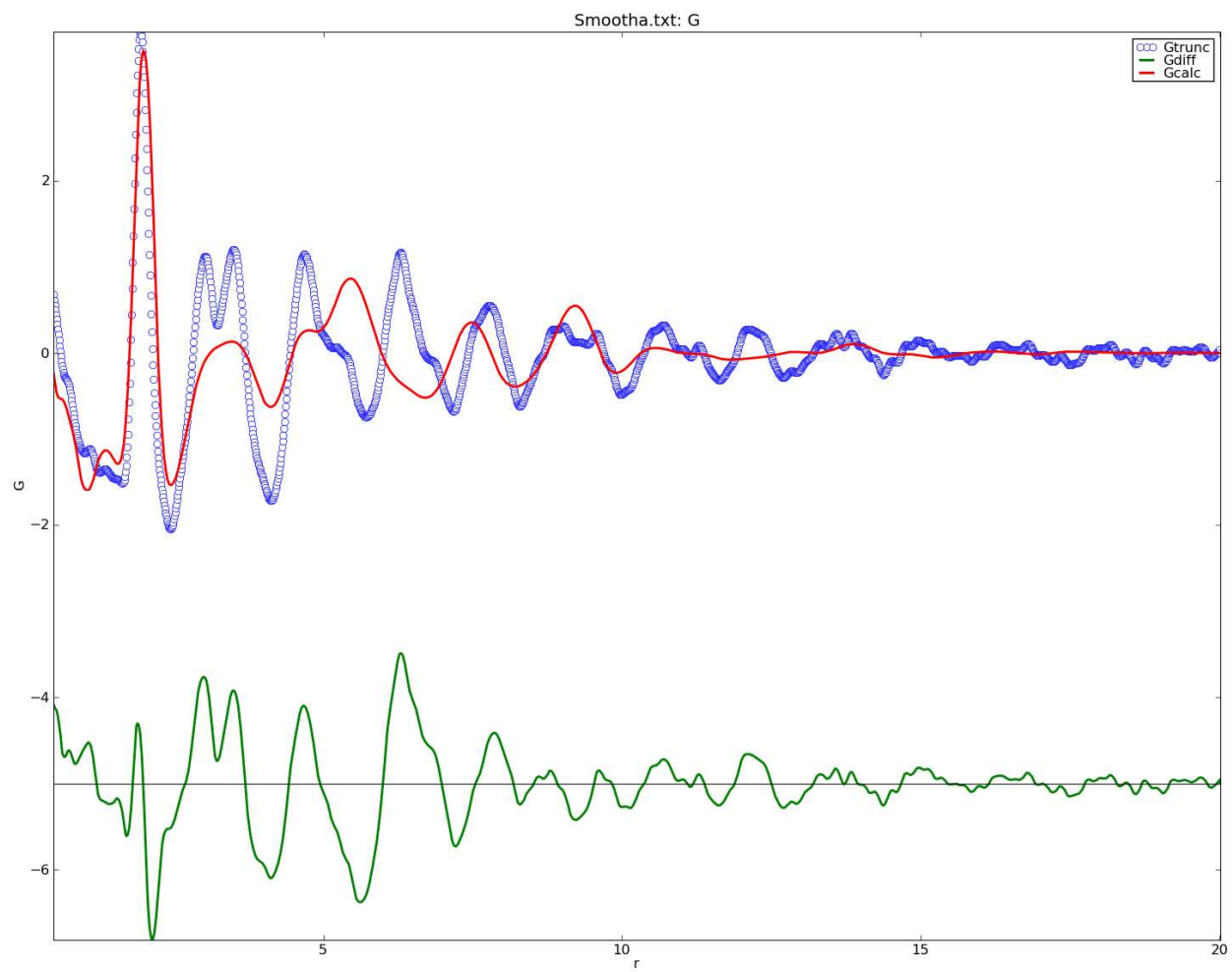**Figure S5, Lepidocrocite** FeOOH,

Refined scale, sratio and tried to refine U_{Fe} and U_O, as they were 0 in the CIF. These did not change from the given values (0.01 & 0.02 respectively). The fit is terrible, as shown below.
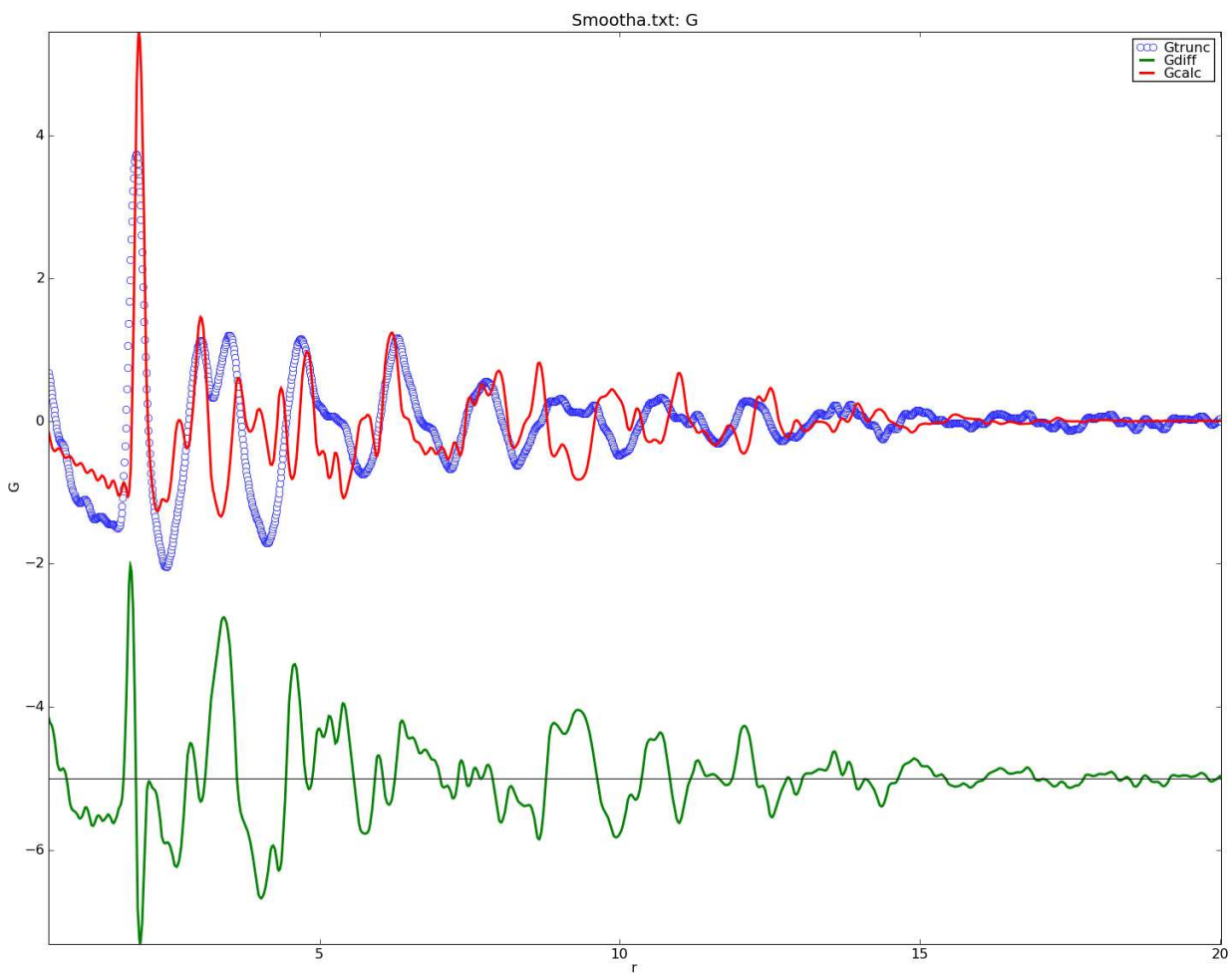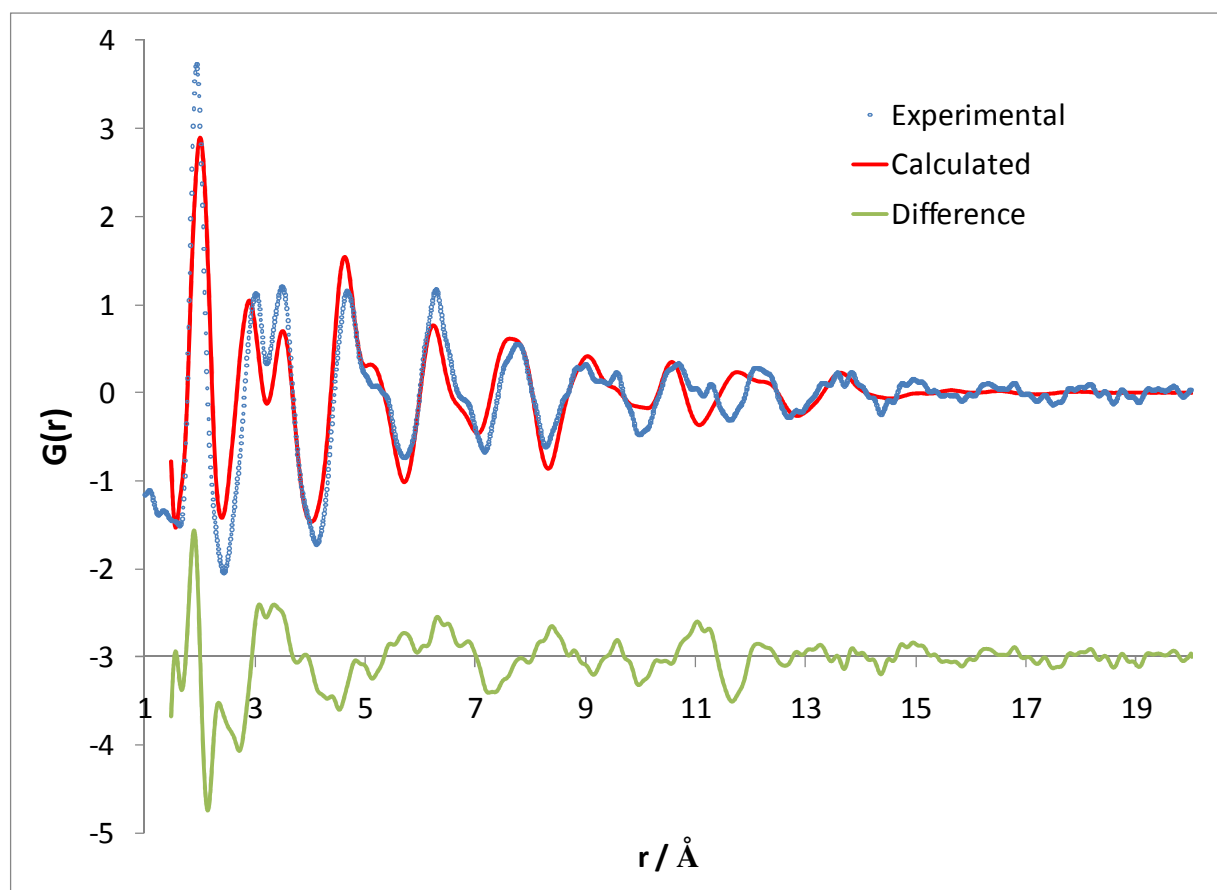
Figure S6, Goethite, α-FeOOH

Refined scale and sratio. With the exception of the first peak, the fit is terrible.

Figure S7. Fit of the dominant defect-free phase from Drits et al. to the neutron diffraction data. The blue circles are the experimental data, the red line the calculated curve and the green curve the difference between them. The fit returned an Rw value of 50%.

Figure S8. Fit of the defective phase from Drits et al. to the neutron diffraction data. The blue circles are the experimental data, the red line the calculated curve and the green curve the difference between them.