

Table 2.1: Interatomic distances, Δr , and σ^2 of W-bearing goethite fit to sample GR_{G-1}, BF-20, SYN-goe_{0.05-1.6,70°C} and SYN-goe_{0.05,25°C}.

GR _{G-1}				BF-20				SYN-goe _{0.05,70°C}				SYN-goe _{0.05,25°C}			
path	N	R [Å]	σ^2	path	N	R [Å]	σ^2	path	N	R [Å]	σ^2	path	N	R [Å]	σ^2
W-O	4	1.928±0.006	0,008	W-O	4	1.774±0.009	0,007	W-O	4	1.812±0.005	0,007	W-O	4	1.781±0.001	0,007
W-O	2	2.100±0.010	0,008	W-O	2	2.100±0.020	0,007	W-O	2	2.120±0.010	0,007	W-O	2	2.120±0.010	0,007
W-Fe	1	2.940±0.030	0,012	W-Fe	1	2.857±0.009	0,015	W-Fe	1	2.980±0.020	0,010	W-Fe	1	2.870±0.001	0,015
W-O	1	3.360±0.020	0,012	W-O	1	3.350±0.020	0,015	W-O	1	3.360±0.010	0,010	W-O	1	3.370±0.020	0,015
W-Fe	1	3.430±0.020	0,012	W-Fe	1	3.430±0.020	0,015	W-Fe	1	3.440±0.010	0,010	W-Fe	1	3.440±0.020	0,015
W-Fe	4	3.570±0.020	0,012	W-Fe	4	3.570±0.020	0,015	W-Fe	4	3.580±0.010	0,010	W-Fe	4	3.580±0.020	0,015
$\Delta E_0 = 1.7$, $N_{var} = 15$, $N_{ind} = 20.2$, $R = 0.025$, k range = 3.6-11.6, R range = 1-4, window type: Hanning				$\Delta E_0 = -0.7$, $N_{var} = 14$, $N_{ind} = 18.77$, $R = 0.017$, k range = 2.5-10, R range = 1-4, window type: Hanning				$\Delta E_0 = 2.5$, $N_{var} = 15$, $N_{ind} = 21.3$, $R = 0.022$, k range = 3-11.5, R range = 1-4, window type: Hanning				$\Delta E_0 = 1.2$, $N_{var} = 14$, $N_{ind} = 21.3$, $R = 0.017$, k range = 2.5-11, R range = 1-4, window type: Hanning			

Table 2.2: Interatomic distances, Δr , and σ^2 of W-bearing hematite fit to sample BF-11, BF-26 and SYN-hem_{0.05-1.6}.

BF-11				BF-26				SYN-hem _{1.6}			
path	N	R [\AA]	σ^2	path	N	R [\AA]	σ^2	path	N	R [\AA]	σ^2
W-O	4	1.822±0.004	0,007	W-O	4	1.823±0.005	0,008	W-O	4	1.845±0.00	
W-O	2	2.100±0.008	0,007	W-O	2	2.090±0.010	0,008			4	0,006
W-Fe	2	3.058±0.006	0,010	W-Fe	2	3.071±0.005	0,010	W-O	2	2.087±0.00	0,006
W-Fe	3	3.451±0.006	0,010	W-Fe	3	3.464±0.005	0,010	W-		9	
W-O	2	3.382±0.008	0,010	W-O	2	3.380±0.010	0,010	Fe	2	3.059±0.00	0,009
W-O	1	3.382±0.008	0,010	W-O	1	3.380±0.010	0,010	5			
W-O	3	3.473±0.004	0,010	W-O	3	3.480±0.005	0,012	W-		5	0,009
W-Fe	3	3.581±0.004	0,010	W-Fe	3	3.590±0.005	0,012	Fe	3	3.452±0.00	
W-Fe	3	3.689±0.008	0,010	W-Fe	3	3.680±0.010	0,012	5			
W-O	3	3.769±0.008	0,010	W-O	3	3.670±0.005	0,012	3.487±0.00			
W-Fe	1	3.969±0.008	0,010	W-Fe	1	3.960±0.010	0,012	W-O	2	5	0,009
W-O	3	4.119±0.008	0,010	W-O	3	4.110±0.010	0,012	3.487±0.00			
W-O	2	4.271±0.004	0,010	W-O	2	4.279±0.005	0,012	5			
W-O	1	4.272±0.004	0,010	W-O	1	4.279±0.005	0,012	3.587±0.00			
$\Delta E_0 = 5.2$, $N_{\text{var}} = 14$, $N_{\text{ind}} = 22.5$, $R = 0.015$, k range = 2.5-11.5, R range = 1-4, window type: Hanning				$\Delta E_0 = 6.6$, $N_{\text{var}} = 15$, $N_{\text{ind}} = 21.3$, $R = 0.019$, k range = 2.5-11, R range = 1-4, window type: Hanning				W-O	3	9	0,013
								W-		3.605±0.00	
								Fe	3	4	0,013
								W-		3.676±0.00	
								Fe	3	9	0,013
										3.685±0.00	
								W-O	3	4	0,013
								W-		3.885±0.00	
								Fe	1	4	0,013
										4.107±0.00	
								W-O	3	9	0,013
										4.366±0.00	
								W-O	2	9	0,013
										4.294±0.00	
								W-O	1	4	0,013
								$\Delta E_0 = 8.9$, $N_{\text{var}} = 15$, $N_{\text{ind}} = 23.8$, $R = 0.018$, k range = 2.5-12, R range = 1-4, window type: Hanning			