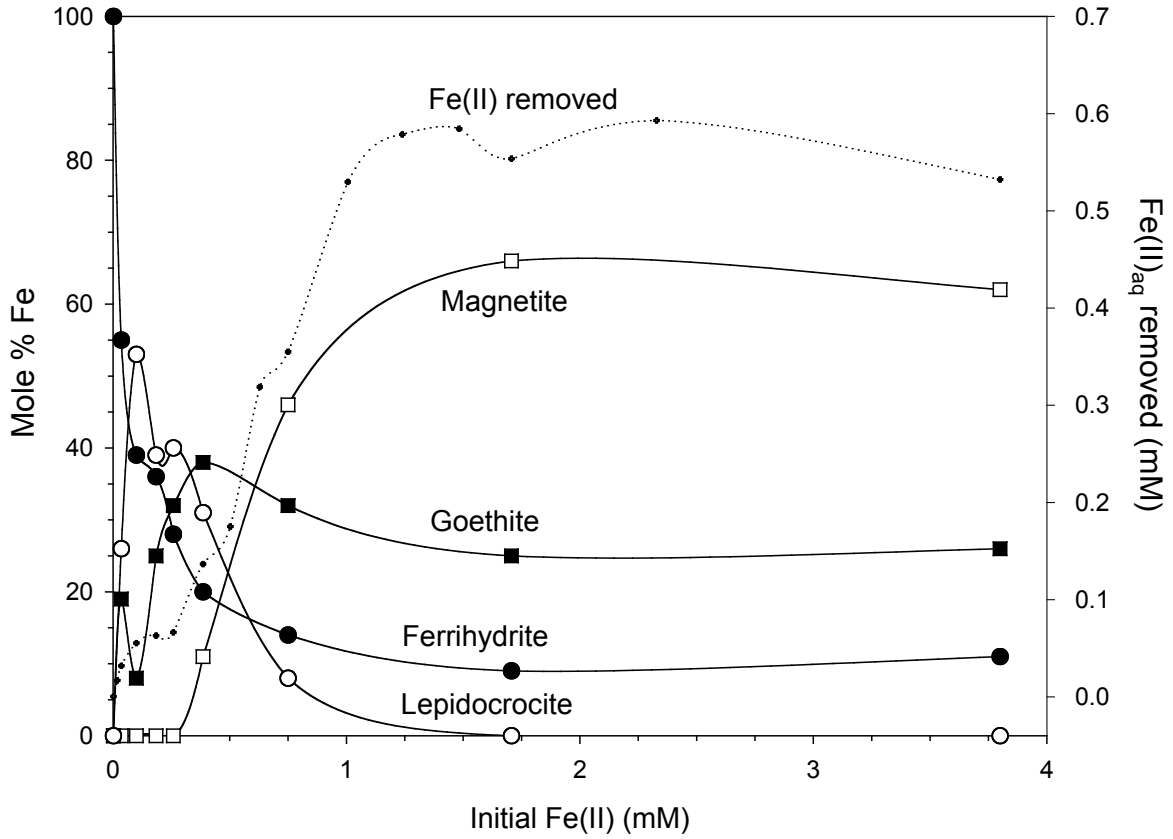
Supporting Information

Competing Fe(II)-induced mineralization pathways of ferrihydrite

Colleen Hansel, Shawn Benner, and Scott Fendorf

Number of pages: 3
Number of figures: 1
Number of tables: 1



Supporting Figure S1. Secondary mineralization of ferrihydrite as a function of initial Fe(II) concentration (modified from Hansel et al., 2003). Reactions involved the addition of 0 to 4.6 mM ferrous chloride to 2-line ferrihydrite-coated sand for 9 d (pH 7.2). Percentages were determined from linear combination fits of k^3-weighted Fe EXAFS spectra (k=1-14) and values are ±5% with a detection limit of ca. 5%.

Substrate*	Fe(II) (mM)	Ligand	Buffer (10 mM)	Time (h)	pH	2L-Fhy-sand†	Goethite	Lepidocrocite	Magnetite
						----------	%	----------	
Ferrihydrite						100	0	0	0
	0.2	Cl	PIPES	2	7	84	1	15	0
				38	7	9	4	87	0
				132	7	6	8	86	0
				120	8	11	8	57	24
	0.2	SO_4	PIPES	2	7	41	11	48	0
				5	7	14	30	56	0
				38	7	5	45	50	0
				132	7	7	46	47	0
	0.2	SO_4	Bicarbonate	132	7	44	56	0	0
	2.0	Cl	PIPES	2	7	30	7	59	4
				6	7	26	10	58	6
				12	7	13	14	63	10
				34	7	22	16	55	7
				120	7	21	13	27	39
				216	7	9	25	0	66
				120	5	66	12	21	0
				120	6	31	0	69	0
				120	7	33	0	36	31
				120	8	8	0	0	92
	2.0	SO_4	PIPES	2	7	33	59	8	0
				5	7	28	72	0	0
				12	7	28	72	0	0
				38	7	23	68	0	8
				132	7	18	55	0	27
	2.0	SO_4	Bicarbonate	132	7	30	70	0	0
	0.04	Cl	PIPES	216	7	55	19	26	0
	0.10			216	7	39	8	53	0
	0.18			216	7	36	25	39	0
	0.26			216	7	28	32	40	0
	0.39			216	7	20	38	31	11
	0.75			216	7	14	32	8	46
	1.71			216	7	9	25	0	66
	3.80			216	7	11	26	0	62
Goethite						29	71	0	0
	2.0	SO_4	PIPES	216	7	31	69	0	0
Lepidocrocite						2		98	
	2.0	Cl	PIPES	192	7	8	4	88	0
	2.0	Cl	Bicarbonate	192	7	0	16	84	0
	0.2	SO_4	PIPES	192	7	1	4	95	0
	0.2	SO_4	Bicarbonate	192	7	0	4	96	0
	2.0	SO_4	PIPES	192	7	8	32	60	0
	2.0	SO_4	Bicarbonate	192	7	0	11	89	0

standard deviation for mineral percentages is ±5%; detection limit is 5%
*initial substrates provided as Fe(III) hydroxide-coated sand (1 wt % Fe)
†2L-Fhy-sand = 2-line ferrihydrite-coated Si sand (starting material)

Supporting Table S1. Secondary mineralization of ferrihydrite as a function of time, initial Fe(II) concentration, ligand, and pH. Percentages were determined from linear combination fits of k^3-weighted Fe EXAFS spectra (k=1-14). All percents are shown, yet please note the detection limit is ~5% for minor phases.