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8 Apêndice

Tabela 8.1 - Dados cristalográficos dos óxidos e hidróxidos de ferro.

Compound	*Crystallographic system*	*Space group*	*Stacking of close packed anions*	*Unit cell dimensions nm*				*Z*
				a	*b*	*c*	*β°*	
Goethite*	Orthorhombic	Pnma	ABAB [001]	0.9956	0.30215	0.4608		4
Lepidocrocite*	Orthorhombic	Bbmm	ABCABC [015]	0.3071	1.2520	0.3873		4
Akaganéite	Monoclinic	I2/m	bcc	1.056	0.3031	1.0483	90.63	8
Schwertmannite	Tetragonal	P4/m		1.066		0.604		
Feroxyhyte	Hexagonal	P3ml	ABAB [001]	0.293		0.456		2
δ-FeOOH	Hexagonal	P3ml	ABAB [001]	0.293		0.449		1
HP FeOOH	Orthorhombic	$Pn2_1m$		0.4932	0.4432	0.2994		2
Ferrihydrite	Hexagonal	P31c; P3	ABAB [001]	0.2955		0.937		4
Hematite	Hexagonal (Rhombohedral)	$R\bar{3}c$	ABAB [001]	0.5034		1.3752		6
Magnetite	Cubic	Fd3m	ABCABC [111]	0.8396				8
Maghemite	Cubic	$P4_332$	ABCABC [111]	0.83474				8
	Tetragonal	$P4_12_12$		0.8347		2.501		24
Wüstite	Cubic	Fm3m		0.4302 (high Fe) 0.4275 (low Fe)				
ε-Fe_2O_3	Orthorhombic	$Pna2_1$		0.5095	0.879	0.9437		8
$Fe(OH)_2$	Hexagonal	P3ml		0.3262		0.4596		1
Bernalite	Orthorhombic	Immm		0.7544	0.7560	0.7558		8

Tabela 8.2 - Parâmetros Mössbauer dos óxidos e hidróxidos de ferro.

Oxide	*Recording temperature K*	*Isomer shift δ mm s⁻¹*	*Quadrupole splitting ΔE_Q mm s⁻¹*	*Hyperfine field B_{hf} T*
Goethite	295	0.37	–0.26	38.0
	4.2	0.48	–0.25	50.6
Lepidocrocite	294	0.37	0.53	–
	4.2	0.47	0.02	45.8
	4.2	0.25	0.02	45.4[g)]

Oxide	*Recording temperature K*	*Isomer shift δ mm s⁻¹*	*Quadrupole splitting ΔE_Q mm s⁻¹*	*Hyperfine field B_hf T*
Akaganéite	295	0.38	0.55	–
		0.37	0.95	–
	4.2	0.49	–0.02	48.9
			–0.24	47.8
			–0.81	47.3
Schwertmannite	295	0.39	0.64	–
	4.2	0.49	–0.37	45.6
δ-FeOOH	295	0.45	0.12	35
	4.2			52.5
HP FeOOH	480	0.03	–0.13	
	295	0.37	–0.13	35.2
	10	0.49	–0.118	47.2
Feroxyhyte	295 [d]	0.37	–0.06	41
	4	0.48	~0	53
			~0	52
Ferrihydrite, 6-line	292	0.24	0.72	–
	4.2	0.25	–0.06	50
Ferrihydrite, 2-line	295	0.24	0.79	–
	4.2	0.24	–0.01	47
Bernalite [a]	295	0.382	–0.006	43.1
	4.2		≤ I0.01I	56.0 [e]
Hematite	295	0.37	–0.197	51.75
	4.2	0.49	0.41	54.17
ε-Fe_2O_3	295	0.21	–0.07	26.2
		0.38	–0.00	39.5
		0.39	–0.06	45.0
		0.37	–0.19	45.2
Magnetite	295	0.26	≤ I0.02I	49
		0.67	0.00	46
Maghemite [b]	295	0.23	≤ I0.02I	50.0
		0.35		50.0
	4.2	0.40	≤ I0.02I	52.0
		0.48	≤ I0.02I	53.0
Wüstite	295	0.95	0.44	–
		0.90	0.79	–
Green Rust -SO_4 [f]	15	~1.3; ~0.5	~2.8; 0.4	–
$Fe(OH)_2$ [c]	300	1.05	2.98	
	4.2	1.4	3.06	~20 [d]

Tabela 8.3 - Coordenadas atômicas dos óxidos e hidróxidos de ferro.

Oxide		*Atomic coordinates*			*Ref.*
		x	*y*	*z*	
Goethite	Fe	0.145	1/4	–0.045	1
	O_1	–0.199	1/4	0.288	
	O_2	–0.053	1/4	–0.198	
	H	–0.08	1/4	–0.38	
Lepidocrocite	Fe	0	–0.3137	1/4	2
	O_1	0	0.2842	1/4	
	O_2	0	0.0724	1/4	
	H	0	0.514	0.366	
Akaganéite	Fe_1	0.858	0	0.341	3
	Fe_2	0.339	0	0.141	
	O_1	0.663	0	0.290	
	O_2	0.657	0	0.030	
	O_3	0.293	0	0.357	
	O_4	0.039	0	0.332	
	Cl	0	0	0	
Feroxyhyte	Fe_1	0	0	0	4
	Fe_2	0	0	1/4	
	O	1/3	2/3	0.246	
	H	1/3	2/3	0.510	
Hematite	Fe	0	0	0.3553	5
	O	0.3059	0	1/4	
Ferrihydrite, 6-line					6
Defect-free phase	Fe	1/3	2/3	0.136	
	O,OH_1	0	0	0	
	O,OH_2	2/3	1/3	1/4	
Defect phase	Fe_1	1/3	2/3	0.163	
	Fe_2	1/3	2/3	0.337	
	Fe_3	1/3	2/3	0.663	
	Fe_4	1/3	2/3	0.837	
	O,OH_1	0	0	0	
	O,OH_2	2/3	2/3	1/2	
Magnetite	Fe_1	1/8	1/8	1/8	7
	Fe_2	1/2	1/2	1/2	
	O	0.25468	0.25468	0.25468	
Maghemite	Fe_1	0.9921	0.9921	0.9921	8
$P4_332$	Fe_2	0.8650	0.6150	7/8	
	Fe_3	3/8	1/8	7/8	
	O_1	0.861	0.861	0.861	
	O_2	0.372	0.377	0.876	
Maghemite	Fe_1	0.7421	0,9921	0.03903	8
$P4_12_12$	Fe_2	0.2579	0.0079	0.2057	
	Fe_3	0.4921	0.7579	0.1224	
	Fe_4	0.6150	0.6150	0	
	Fe_5	0.385	0.385	1/6	
	Fe_6	3/8	0.135	0.08	

Oxide		*Atomic coordinates*			*Ref.*
		x	*y*	*z*	
Maghemite	Fe_7	0.865	5/8	0.0867	
$P4_12_12$	Fe_8	7/8	0.365	0.003	
	Fe_9	1/8	1/8	0	
	O_1	0.611	0.861	–0.0047	
	O_2	0.361	0.889	0.0787	
	O_3	0.389	0.139	0.162	
	O_4	0.122	0.377	0.0003	
	O_5	0.877	0.378	0.0837	
	O_6	0.878	0.623	1/6	
	O_7	0.374	0.628	0.0007	
	O_8	0.128	0.126	0.084	
	O_9	0.626	0.372	0.1673	
	O_{10}	0.373	0.376	0.0843	
	O_{11}	0.624	0.627	0.0843	
	O_{12}	0.124	0.873	0.001	
Wüstite	Fe	0	0	0	9
	O	1/2	1/2	1/2	

Tabela 8.4 - Distancias interplanares de alguns compostos de ferro.

Magnetita (Fe_3O_4)

H	K	L	2Θ/ deg	d / Å
1	1	1	18.287	4.84743
2	2	0	30.080	2.96843
3	1	1	35.431	2.53149
2	2	2	37.062	2.42372
4	0	0	43.059	2.09900
3	3	1	47.145	1.92617
4	2	2	53.418	1.71383
3	3	3	56.944	1.61581
5	1	1	56.944	1.61581
4	4	0	62.530	1.48422
5	3	1	65.746	1.41918
4	4	2	66.799	1.39933

H	K	L	2Θ/ deg	d / Å
6	2	0	70.937	1.32752
5	3	3	73.972	1.28038
6	2	2	74.973	1.26574
4	4	4	78.934	1.21186
7	1	1	81.869	1.17568
5	5	1	81.869	1.17568
6	4	2	86.717	1.12196
7	3	1	89.613	1.09307
5	5	3	89.613	1.09307
8	0	0	94.440	1.04950
7	3	3	97.349	1.02573
6	4	4	98.323	1.01816

Wüstita (FeO)

H	K	L	2Θ/ deg	d / Å
1	1	1	36.135	2.48376
2	0	0	41.969	2.15100
2	2	0	60.855	1.52099

H	K	L	2Θ/ deg	d / Å
3	1	1	72.863	1.29710
2	2	2	76.671	1.24188
4	0	0	91.487	1.07550

Hematita (α-Fe_2O_3)

H	K	L	2Θ/ deg	d / Å
0	1	2	24.152	3.68189
1	0	4	33.159	2.69956
1	1	0	35.641	2.51700
0	0	6	39.277	2.29200
1	1	3	40.869	2.20629
2	0	2	43.519	2.07787
0	2	4	49.470	1.84095
1	1	6	54.071	1.69466
2	1	1	56.176	1.63606
1	2	2	57.465	1.60240
0	1	8	57.591	1.59917
2	1	4	62.450	1.48591
3	0	0	64.021	1.45319
1	2	5	66.043	1.41351
2	0	8	69.596	1.34978
1	0	10	71.937	1.31150
1	1	9	72.278	1.30616
2	1	7	75.200	1.26248

H	K	L	2Θ/ deg	d / Å
2	2	0	75.480	1.25850
3	0	6	77.752	1.22730
0	3	6	77.752	1.22730
2	2	3	78.799	1.21359
1	3	1	79.513	1.20448
3	1	2	80.608	1.19086
1	2	8	80.717	1.18953
0	2	10	82.950	1.16308
0	0	12	84.468	1.14600
1	3	4	84.958	1.14064
3	1	5	88.200	1.10689
2	2	6	88.578	1.10314
0	4	2	91.383	1.07645
2	1	10	93.703	1.05581
1	1	12	95.217	1.04298
4	0	4	95.707	1.03894
1	3	7	96.846	1.02973

Maghemita C (γ-Fe_2O_3)

H	K	L	2Θ/ deg	d / Å
1	1	0	14.997	5.90250
1	1	1	18.395	4.81937
2	1	0	23.816	3.73307
2	1	1	26.128	3.40781
2	2	0	30.260	2.95125
2	2	1	32.143	2.78247
3	1	0	33.933	2.63968
3	1	1	35.644	2.51684
2	2	2	37.286	2.40969
3	2	0	38.868	2.31515
3	2	1	40.398	2.23094
4	0	0	43.323	2.08685
4	1	0	44.727	2.02454
3	2	2	44.727	2.02454
3	3	0	46.097	1.96750
4	1	1	46.097	1.96750
3	3	1	47.437	1.91502
4	2	0	48.748	1.86654
4	2	1	50.033	1.82155
3	3	2	51.295	1.77967
4	2	2	53.754	1.70391
4	3	0	54.955	1.66948
5	1	0	56.138	1.63706
4	3	1	56.138	1.63706
3	3	3	57.306	1.60646
5	1	1	57.306	1.60646
4	3	2	59.596	1.55007
5	2	0	59.596	1.55007
5	2	1	60.721	1.52402
4	4	0	62.935	1.47563
4	4	1	64.026	1.45310
5	2	2	64.026	1.45310
4	3	3	65.106	1.43157
5	3	0	65.106	1.43157
5	3	1	66.177	1.41097
4	4	2	67.240	1.39123
6	1	0	68.294	1.37230
5	3	2	69.341	1.35413
6	1	1	69.341	1.35413
6	2	0	71.413	1.31984
4	4	3	72.439	1.30364

H	K	L	2Θ/ deg	d / Å
6	2	1	72.439	1.30364
5	4	0	72.439	1.30364
5	4	1	73.460	1.28803
5	3	3	74.475	1.27297
6	2	2	75.485	1.25842
6	3	0	76.491	1.24436
5	4	2	76.491	1.24436
6	3	1	77.493	1.23076
4	4	4	79.485	1.20484
6	3	2	80.476	1.19249
7	1	0	81.464	1.18050
5	5	0	81.464	1.18050
5	4	3	81.464	1.18050
5	5	1	82.449	1.16887
7	1	1	82.449	1.16887
6	4	0	83.432	1.15758
7	2	0	84.414	1.14660
6	4	1	84.414	1.14660
5	5	2	85.393	1.13594
7	2	1	85.393	1.13594
6	3	3	85.393	1.13594
6	4	2	87.349	1.11547
5	4	4	88.326	1.10564
7	2	2	88.326	1.10564
7	3	0	89.302	1.09607
5	5	3	90.277	1.08674
7	3	1	90.277	1.08674
6	4	3	92.230	1.06878
6	5	0	92.230	1.06878
7	3	2	93.207	1.06012
6	5	1	93.207	1.06012
8	0	0	95.164	1.04342
8	1	0	96.144	1.03537
6	5	2	96.144	1.03537
7	4	0	96.144	1.03537
5	5	4	97.127	1.02749
8	1	1	97.127	1.02749
7	4	1	97.127	1.02749
7	3	3	98.111	1.01980
8	2	0	99.098	1.01227
6	4	4	99.098	1.01227

Goethita (α-FeOOH)

H	K	L	2Θ/ deg	d / Å
2	0	0	17.804	4.97800
1	0	1	21.229	4.18181
2	0	1	26.334	3.38160
3	0	1	33.242	2.69296
2	1	0	34.702	2.58294
0	1	1	35.499	2.52675
4	0	0	36.056	2.48900
1	1	1	36.664	2.44910
0	0	2	39.064	2.30400
2	1	1	39.983	2.25312
1	0	2	40.140	2.24468
4	0	1	41.188	2.18995
2	0	2	43.235	2.09090
3	1	1	45.059	2.01037
4	1	0	47.277	1.92111
3	0	2	48.034	1.89260
5	0	1	49.849	1.82785
1	1	2	50.618	1.80186
4	1	1	51.496	1.77318
2	1	2	53.233	1.71937
4	0	2	54.205	1.69080
6	0	0	55.320	1.65933
3	1	2	57.404	1.60393
5	1	1	59.015	1.56394
6	0	1	59.129	1.56120
1	0	3	60.986	1.51804
0	2	0	61.311	1.51075
5	0	2	61.501	1.50654
4	1	2	62.942	1.47549
2	0	3	63.313	1.46772
6	1	0	63.959	1.45444
2	2	0	64.395	1.44564
1	2	1	65.658	1.42087
3	0	3	67.092	1.39394
6	1	1	67.473	1.38699
2	2	1	67.897	1.37935
0	1	3	68.468	1.36923
7	0	1	69.055	1.35902
1	1	3	69.204	1.35646
5	1	2	69.687	1.34824
6	0	2	69.791	1.34648
2	1	3	71.390	1.32020
3	2	1	71.554	1.31758

H	K	L	2Θ/ deg	d / Å
4	0	3	72.215	1.30714
4	2	0	73.232	1.29147
3	1	3	74.974	1.26573
0	2	2	75.138	1.26337
1	2	2	75.846	1.25332
8	0	0	76.481	1.24450
4	2	1	76.550	1.24355
7	1	1	76.851	1.23942
6	1	2	77.558	1.22989
2	2	2	77.959	1.22455
5	0	3	78.598	1.21620
7	0	2	79.059	1.21026
8	0	1	79.754	1.20145
4	1	3	79.895	1.19969
3	2	2	81.446	1.18071
5	2	1	82.828	1.16448
0	0	4	83.928	1.15200
8	1	0	84.043	1.15071
1	0	4	84.617	1.14436
5	1	3	86.118	1.12823
6	0	3	86.216	1.12720
4	2	2	86.277	1.12656
7	1	2	86.571	1.12348
2	0	4	86.681	1.12234
6	2	0	87.189	1.11711
8	1	1	87.255	1.11643
8	0	2	89.415	1.09497
3	0	4	90.113	1.08830
6	2	1	90.392	1.08566
9	0	1	91.470	1.07566
1	2	3	92.001	1.07083
1	1	4	92.073	1.07018
5	2	2	92.454	1.06677
6	1	3	93.669	1.05610
2	2	3	94.062	1.05272
2	1	4	94.134	1.05210
4	0	4	94.921	1.04545
7	0	3	95.143	1.04360
8	1	2	96.879	1.02946
3	2	3	97.510	1.02447
3	1	4	97.583	1.02390
9	1	1	98.954	1.01336
7	2	1	99.351	1.01037

Akaganeita (β-FeOOH)

H	K	L	2Θ/ deg	d / Å
2	0	0	16.778	5.28000
0	0	2	16.902	5.24150
-2	0	1	18.803	4.71563
2	0	1	18.803	4.71563
2	0	2	23.902	3.71984
-2	0	2	23.902	3.71984
0	0	3	25.470	3.49433
-2	0	3	30.656	2.91398
2	0	3	30.656	2.91398
1	1	0	30.663	2.91337
1	1	1	31.855	2.80698
-1	1	1	31.855	2.80698
4	0	0	33.929	2.64000
0	0	4	34.186	2.62075
-4	0	1	35.022	2.56007
4	0	1	35.022	2.56007
1	1	2	35.216	2.54645
-1	1	2	35.216	2.54645
-4	0	2	38.137	2.35781
4	0	2	38.137	2.35781
-2	0	4	38.312	2.34748
2	0	4	38.312	2.34748
3	1	0	39.191	2.29683
-3	1	1	40.160	2.24361
3	1	1	40.160	2.24361
-1	1	3	40.271	2.23766
1	1	3	40.271	2.23766
-4	0	3	42.900	2.10642
4	0	3	42.900	2.10642
3	1	2	42.958	2.10372
-3	1	2	42.958	2.10372
0	0	5	43.111	2.09660
2	0	5	46.571	1.94860
-2	0	5	46.571	1.94860
-1	1	4	46.575	1.94841
1	1	4	46.575	1.94841
-3	1	3	47.323	1.91934
3	1	3	47.323	1.91934
4	0	4	48.933	1.85992
-4	0	4	48.933	1.85992
6	0	0	51.911	1.76000
0	0	6	52.321	1.74717
-6	0	1	52.693	1.73571

H	K	L	2Θ/ deg	d / Å
5	1	0	52.787	1.73282
-3	1	4	52.968	1.72734
3	1	4	52.968	1.72734
5	1	1	53.560	1.70962
-5	1	1	53.560	1.70962
1	1	5	53.828	1.70175
-1	1	5	53.828	1.70175
6	0	2	54.992	1.66845
-6	0	2	54.992	1.66845
-2	0	6	55.342	1.65871
2	0	6	55.342	1.65871
-5	1	2	55.835	1.64524
5	1	2	55.835	1.64524
4	0	5	55.961	1.64183
-4	0	5	55.961	1.64183
-6	0	3	58.688	1.57188
6	0	3	58.688	1.57188
-5	1	3	59.497	1.55242
5	1	3	59.497	1.55242
-3	1	5	59.664	1.54848
3	1	5	59.664	1.54848
0	2	0	61.099	1.51550
0	2	1	61.803	1.49991
1	1	6	61.873	1.49838
-1	1	6	61.873	1.49838
0	0	7	61.910	1.49757
-6	0	4	63.634	1.46110
6	0	4	63.634	1.46110
4	0	6	63.834	1.45699
-4	0	6	63.834	1.45699
2	2	0	63.849	1.45668
0	2	2	63.889	1.45587
-5	1	4	64.406	1.44543
5	1	4	64.406	1.44543
2	2	1	64.537	1.44282
-2	2	1	64.537	1.44282
-2	0	7	64.641	1.44074
2	0	7	64.641	1.44074
2	2	2	66.576	1.40349
-2	2	2	66.576	1.40349
3	1	6	67.276	1.39057
-3	1	6	67.276	1.39057
0	2	3	67.287	1.39037

Lepidocrocita (γ-FeOOH)

H	K	L	2Θ/ deg	d / Å
0	2	0	14.136	6.26000
0	2	1	27.051	3.29360
0	4	0	28.494	3.13000
1	1	0	29.934	2.98259
1	3	0	36.290	2.47348
0	4	1	36.893	2.43440
1	1	1	38.049	2.36308
0	6	0	43.327	2.08667
1	3	1	43.371	2.08462
1	5	0	46.772	1.94066
0	0	2	46.879	1.93650
0	2	2	49.212	1.85000
0	6	1	49.584	1.83701
1	5	1	52.715	1.73503
0	4	2	55.777	1.64680
1	1	2	56.623	1.62419
0	8	0	58.971	1.56500
1	7	0	59.788	1.54555
2	0	0	60.220	1.53550
1	3	2	60.687	1.52478
2	2	0	62.200	1.49129
0	8	1	64.128	1.45102
1	7	1	64.907	1.43548
0	6	2	65.733	1.41943
2	2	1	67.215	1.39169
2	4	0	67.942	1.37855
1	5	2	68.380	1.37078
2	4	1	72.757	1.29873

H	K	L	2Θ/ deg	d / Å
1	9	0	74.874	1.26717
0	2	3	75.067	1.26439
0	10	0	75.941	1.25200
2	6	0	77.048	1.23674
0	8	2	78.521	1.21720
1	7	2	79.237	1.20798
1	9	1	79.524	1.20434
2	0	2	79.618	1.20316
0	4	3	80.396	1.19347
0	10	1	80.572	1.19130
1	1	3	81.108	1.18477
2	2	2	81.377	1.18154
2	6	1	81.662	1.17813
1	3	3	84.606	1.14449
2	4	2	86.613	1.12305
0	6	3	89.116	1.09787
2	8	0	89.304	1.09604
1	5	3	91.554	1.07489
1	11	0	92.401	1.06724
1	9	2	93.183	1.06033
2	8	1	93.840	1.05463
0	10	2	94.217	1.05140
0	12	0	95.175	1.04333
2	6	2	95.298	1.04231
1	11	1	96.950	1.02889
3	1	0	98.051	1.02026
0	12	1	99.747	1.00742

Feroxita (δ-FeOOH)

H	K	L	2Θ/ deg	d / Å
0	0	1	19.451	4.56000
1	0	0	35.344	2.53745
0	0	2	39.492	2.28000
1	0	1	40.658	2.21728
0	1	1	40.658	2.21728
0	1	2	54.027	1.69594
1	0	2	54.027	1.69594
0	0	3	60.899	1.52000
1	1	0	63.444	1.46500
1	1	1	67.046	1.39479
0	1	3	72.419	1.30395

H	K	L	2Θ/ deg	d / Å
1	0	3	72.419	1.30395
2	0	0	74.766	1.26873
1	1	2	77.363	1.23250
0	2	1	78.131	1.22230
2	0	1	78.131	1.22230
0	0	4	85.017	1.14000
0	2	2	88.025	1.10864
2	0	2	88.025	1.10864
1	1	3	93.817	1.05482
0	1	4	95.593	1.03987
1	0	4	95.593	1.03987