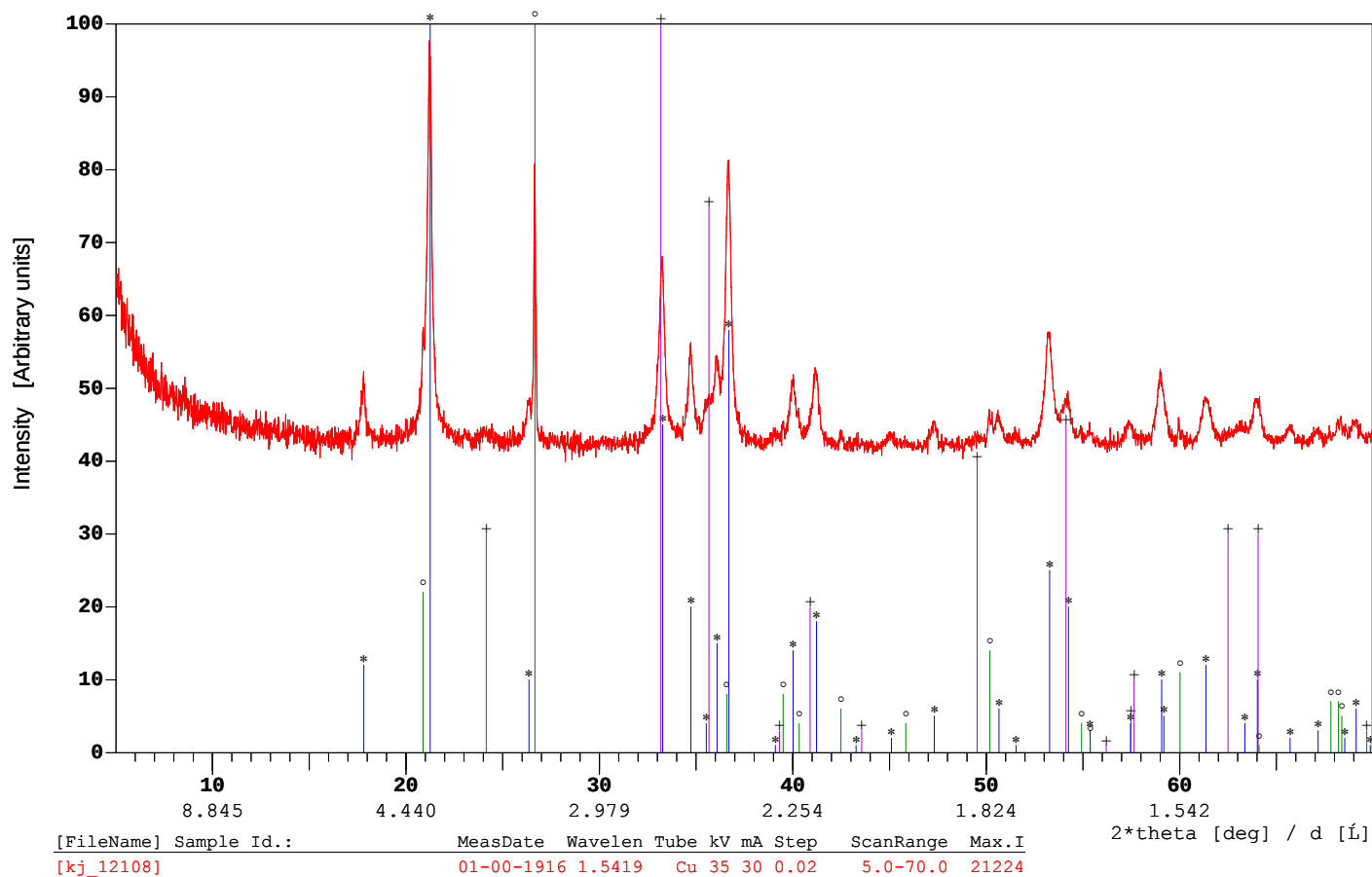


Supplementary materials

XDB dataset



Reference patterns:

*29-0713 Goet Goethite (revised) FeO(OH)
 +33-0664 Hema Hematite (revised) Fe2O3
 °33-1161 Quar Quartz SiO2

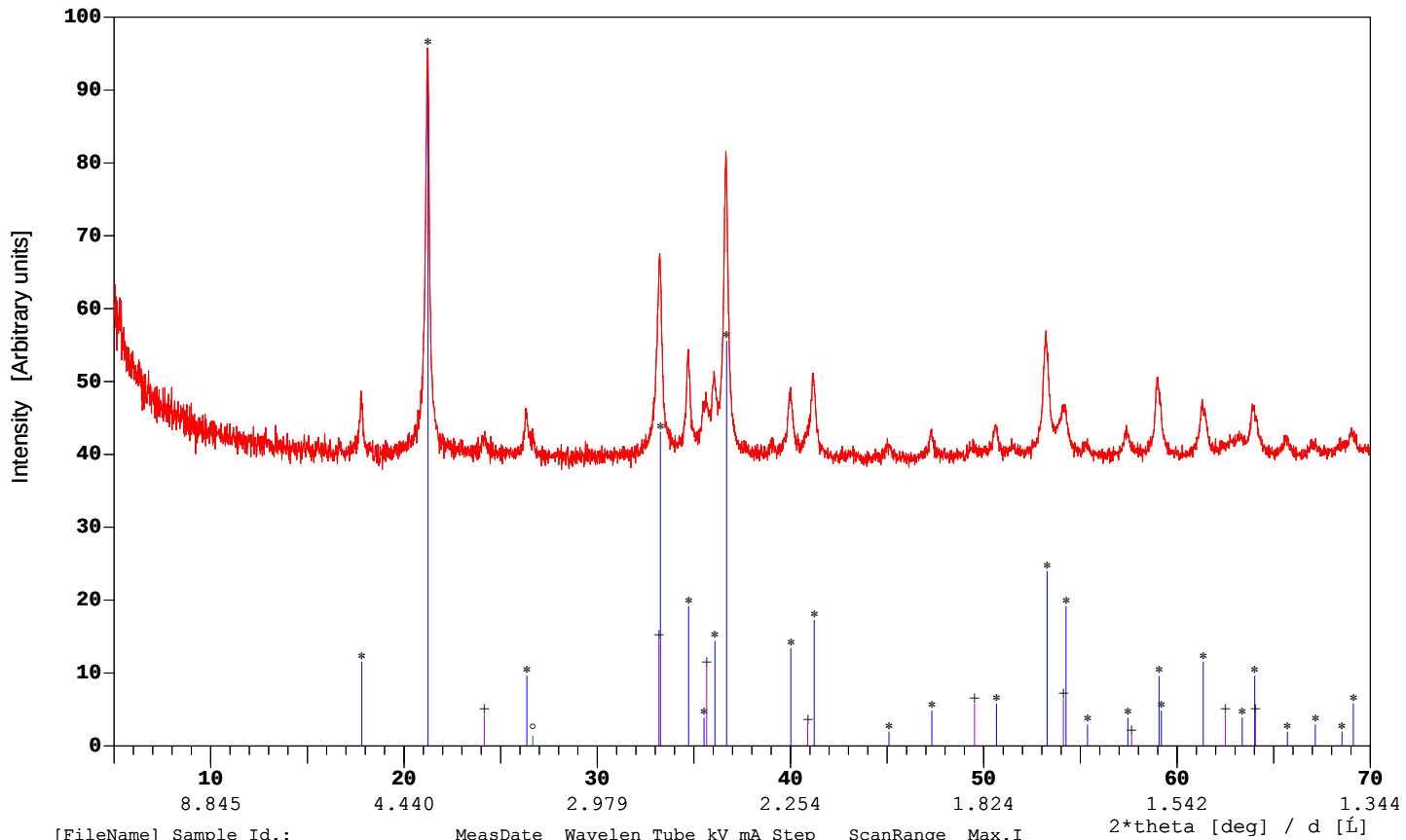
[KJ_12108]

Phase%	SUM	Goet	Hema	Quar	Chem	
	100.00	90.00	5.00	5.00	Anal	Diff
Fe ₂ O ₃ %	85.88	80.88	5.00		57.10	-28.78
SiO ₂ %	5.00			5.00	24.00	19.00
H ₂ O%	9.12	9.12				
LOI %	9.12	9.12	0.00	0.00	8.71	-0.41

Orient.	[r]	1.00	1.00	1.00
Shape	[exp]	1.50	1.50	1.50
FWHM:	[0.10]	0.30	0.35	0.10
xSize	[nm]	49	39	>1000
pSize	[um]	2.0	3.0	5.0
MAC	(CuKa)	197.7	218.9	34.5
I/Ic		1.40	2.60	3.60

Profile R = 0.03
 Chi square = 3.31
 Full Scale (obs) = 21224 counts
 Full Scale (calc) = 21224 counts
 2theta offset = 0.0 deg

XDB



Reference patterns:

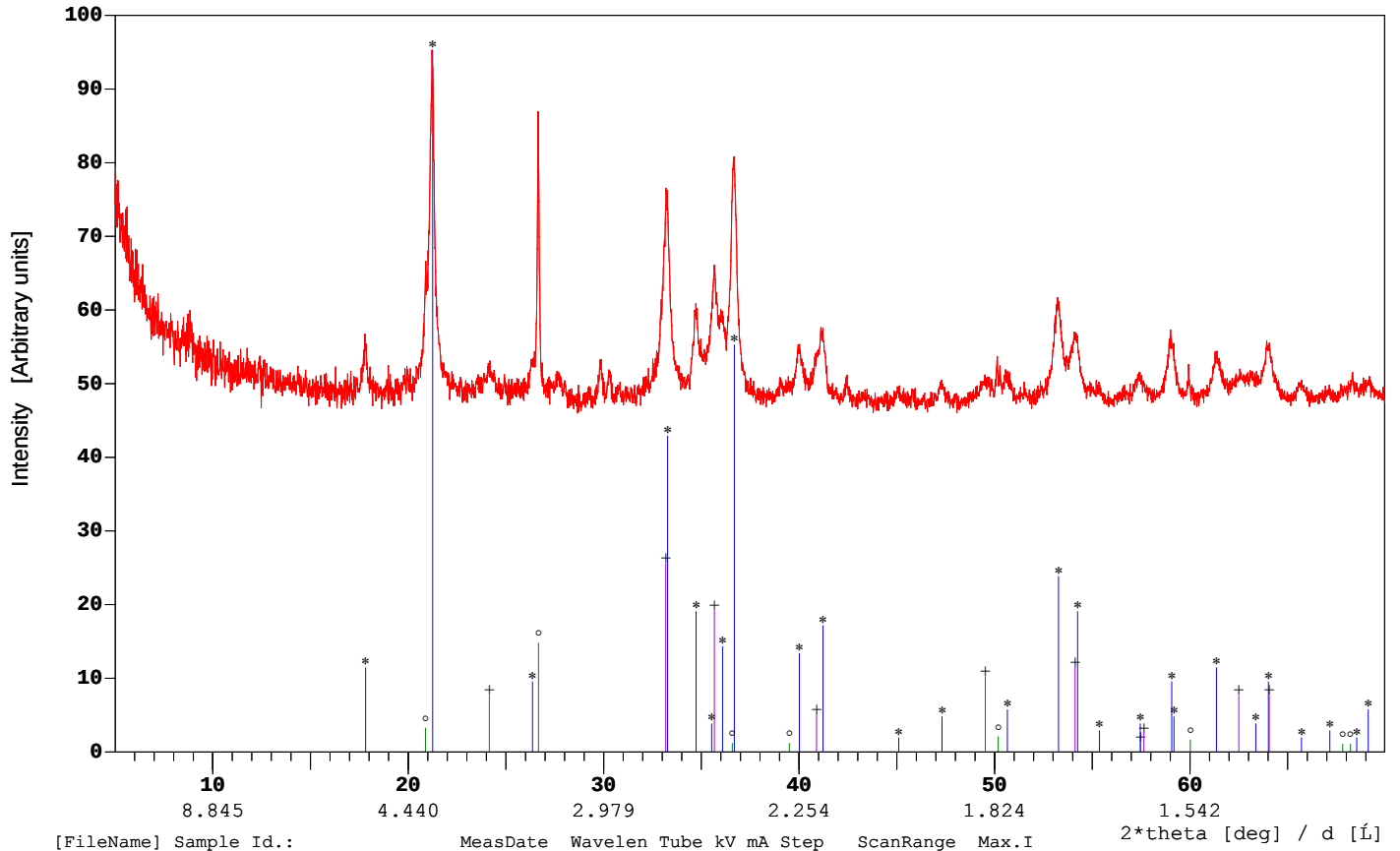
*29-0713 Goet Goethite (revised) FeO(OH)
 +33-0664 Hema Hematite (revised) Fe2O3
 *33-1161 Quar Quartz SiO2

[KJ_12109]

	SUM	Goet	Hema	Quar
Phase%	100.00	92.00	7.50	0.50
Fe ₂ O ₃ %	90.17	82.67	7.50	
SiO ₂ %	0.50			0.50
H ₂ O%	9.33	9.33		
LOI %	9.33	9.33	0.00	0.00
Orient.	[r]	1.00	1.00	1.00
Shape	[exp]	1.50	1.50	1.50
FWHM:	[0.10]	0.30	0.30	0.10
xSize	[nm]	49	49	>1000
pSize	[um]	3.0	3.0	5.0
MAC	(CuKa)	197.7	218.9	34.5
I/Ic		1.40	2.60	3.60

Profile R = 0.03
 Chi square = 3.58
 Full Scale (obs) = 22587 counts
 Full Scale (calc) = 22587 counts
 2theta offset = 0.0 deg

XDB



Reference patterns:

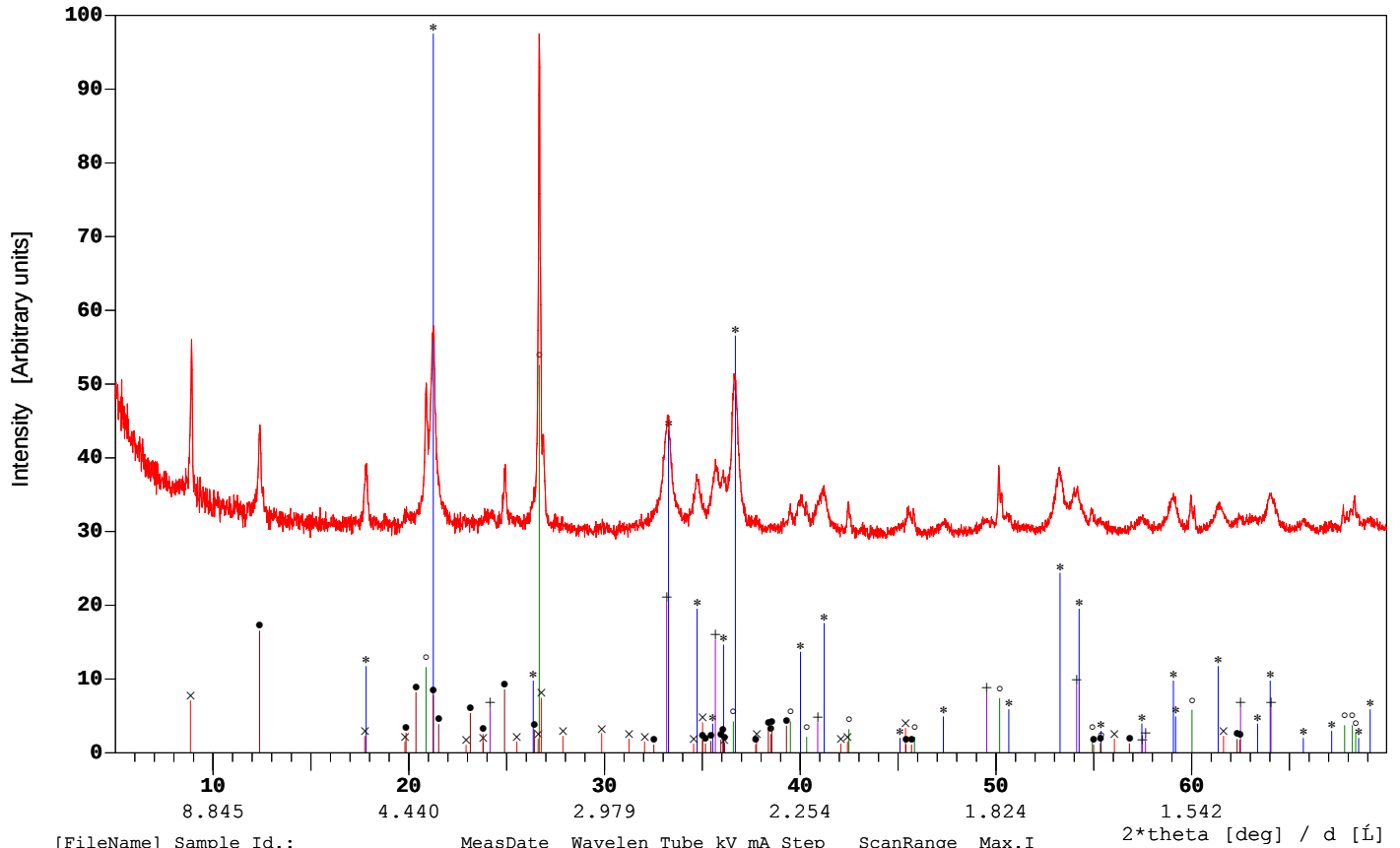
*29-0713 Goet Goethite (revised) FeO(OH)
 +33-0664 Hema Hematite (revised) Fe2O3
 °33-1161 Quar Quartz SiO2

[KJ_12110]

	SUM	Goet	Hema	Quar
Phase%	100.00	83.00	12.00	5.00
Fe ₂ O ₃ %	86.59	74.59	12.00	
SiO ₂ %	5.00			5.00
H ₂ O%	8.41	8.41		
LOI %	8.41	8.41	0.00	0.00
Orient.	[r]	1.00	1.00	1.00
Shape	[exp]	1.50	1.50	1.50
FWHM:	[0.10]	0.30	0.30	0.10
xSize	[nm]	49	49	>1000
pSize	[um]	3.0	3.0	5.0
MAC	(CuKa)	197.7	218.9	34.5
I/Ic		1.40	2.60	3.60

Profile R = 0.03
 Chi square = 3.57
 Full Scale (obs) = 17337 counts
 Full Scale (calc) = 17337 counts
 2theta offset = 0.0 deg

XDB



Reference patterns:

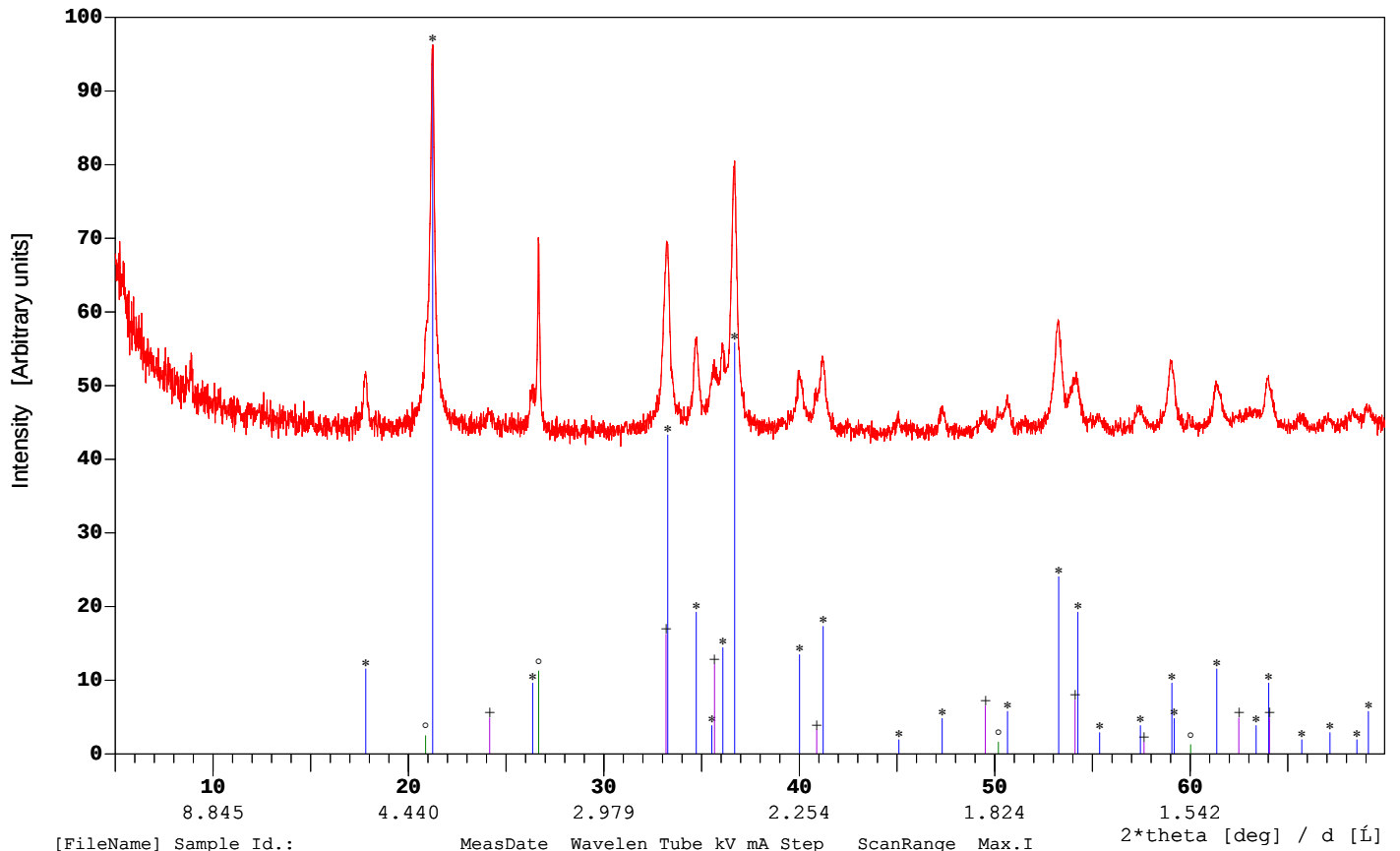
*29-0713 Goet Goethite (revised) FeO(OH)
 +33-0664 Hema Hematite (revised) Fe2O3
 °33-1161 Quar Quartz SiO2
 x06-0263 Musc Muscovite 2M1 KAl2(Si3Al)O10(OH,F)2
 •79-1570 KaoT Kaolinite 1T Al2[Si2O5(OH)4]

[KJ_12111]

	SUM	Goet	Hema	Quar	Musc	KaoT
Phase%	100.00	62.00	7.00	13.00	3.00	15.00
Fe ₂ O ₃ %	62.72	55.72	7.00			
K ₂ O%	0.35				0.35	
SiO ₂ %	21.34			13.00	1.35	6.98
Al ₂ O ₃ %	7.07				1.15	5.92
F%	0.07				0.07	
H ₂ O%	8.48	6.29			0.10	2.09
LOI %	8.48	6.28	0.00	0.00	0.10	2.09
Orient.	[r]	1.00	1.00	1.00	0.50	0.70
Shape	[exp]	1.50	1.50	1.50	1.50	1.50
FWHM:	[0.10]	0.30	0.30	0.10	0.11	0.20
xSize	[nm]	49	49	>1000	987	99
pSize	[um]	3.0	3.0	5.0	3.0	1.0
MAC	(CuKa)	197.7	218.9	34.5	42.3	29.8
I/Ic		1.40	2.60	3.60	2.20	0.98

Profile R = 0.03
 Chi square = 3.90
 Full Scale (obs) = 27343 counts
 Full Scale (calc) = 27343 counts
 2theta offset = 0.0 deg

XDB



Reference patterns:

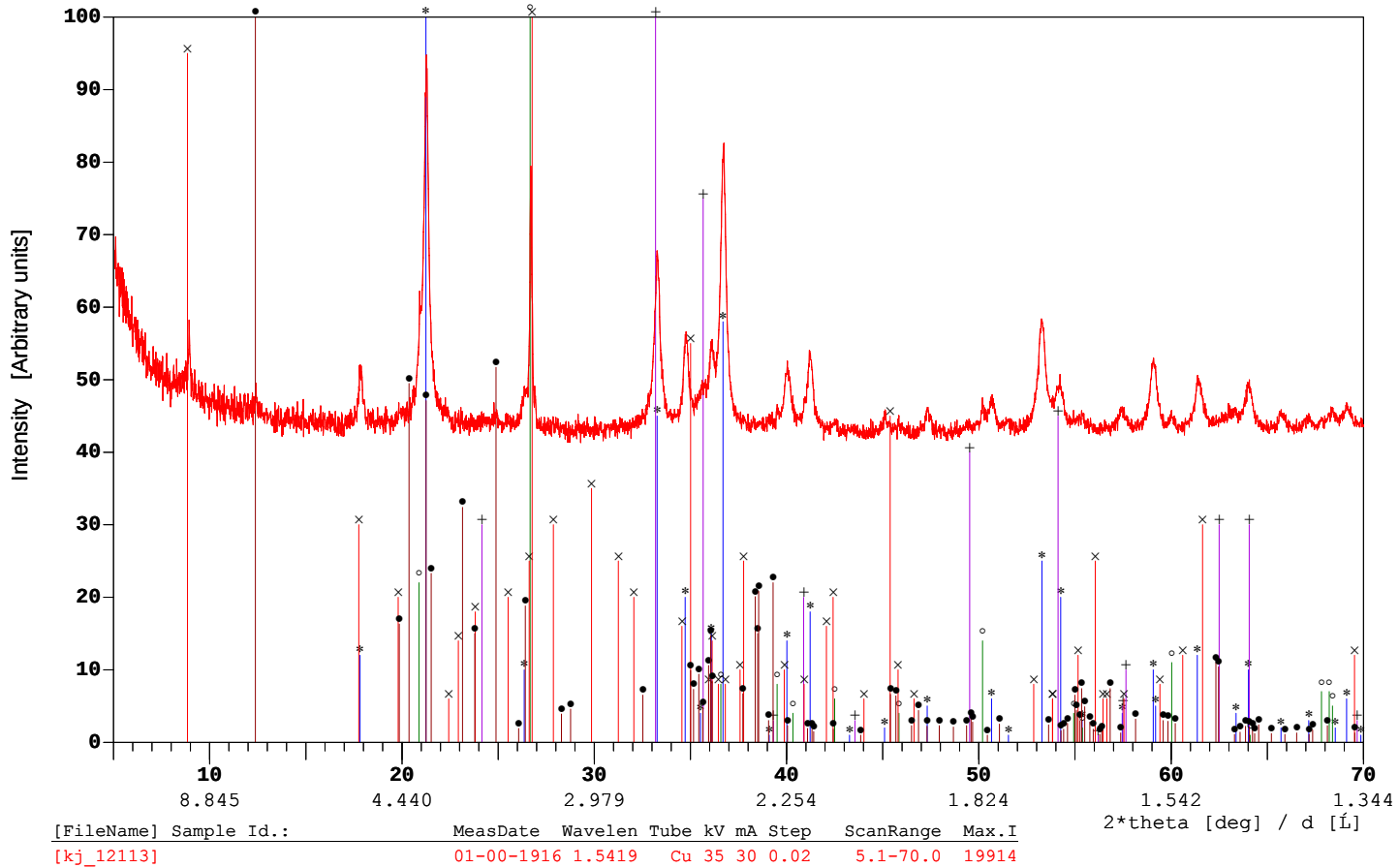
*29-0713 Goet Goethite (revised) FeO(OH)
 +33-0664 Hema Hematite (revised) Fe2O3
 °33-1161 Quar Quartz SiO2

[KJ_12112]

	SUM	Goet	Hema	Quar
Phase%	100.00	88.00	8.00	4.00
Fe ₂ O ₃ %	87.08	79.08	8.00	
SiO ₂ %	4.00			4.00
H ₂ O%	8.92	8.92		
LOI %	8.92	8.92	0.00	0.00
Orient.	[r]	1.00	1.00	1.00
Shape	[exp]	1.50	1.50	1.50
FWHM:	[0.10]	0.30	0.30	0.10
xSize	[nm]	49	49	>1000
pSize	[um]	3.0	3.0	5.0
MAC	(CuKa)	197.7	218.9	34.5
I/Ic		1.40	2.60	3.60

Profile R = 0.02
 Chi square = 3.11
 Full Scale (obs) = 20429 counts
 Full Scale (calc) = 20429 counts
 2theta offset = 0.0 deg

XDB



Reference patterns:

*29-0713 Goet Goethite (revised) FeO(OH)
 +33-0664 Hema Hematite (revised) Fe2O3
 o33-1161 Quar Quartz SiO2
 x06-0263 Musc Muscovite 2M1 KAl2(Si3Al)O10(OH,F)2
 •79-1570 KaoT Kaolinite 1T Al2[Si2O5(OH)4]

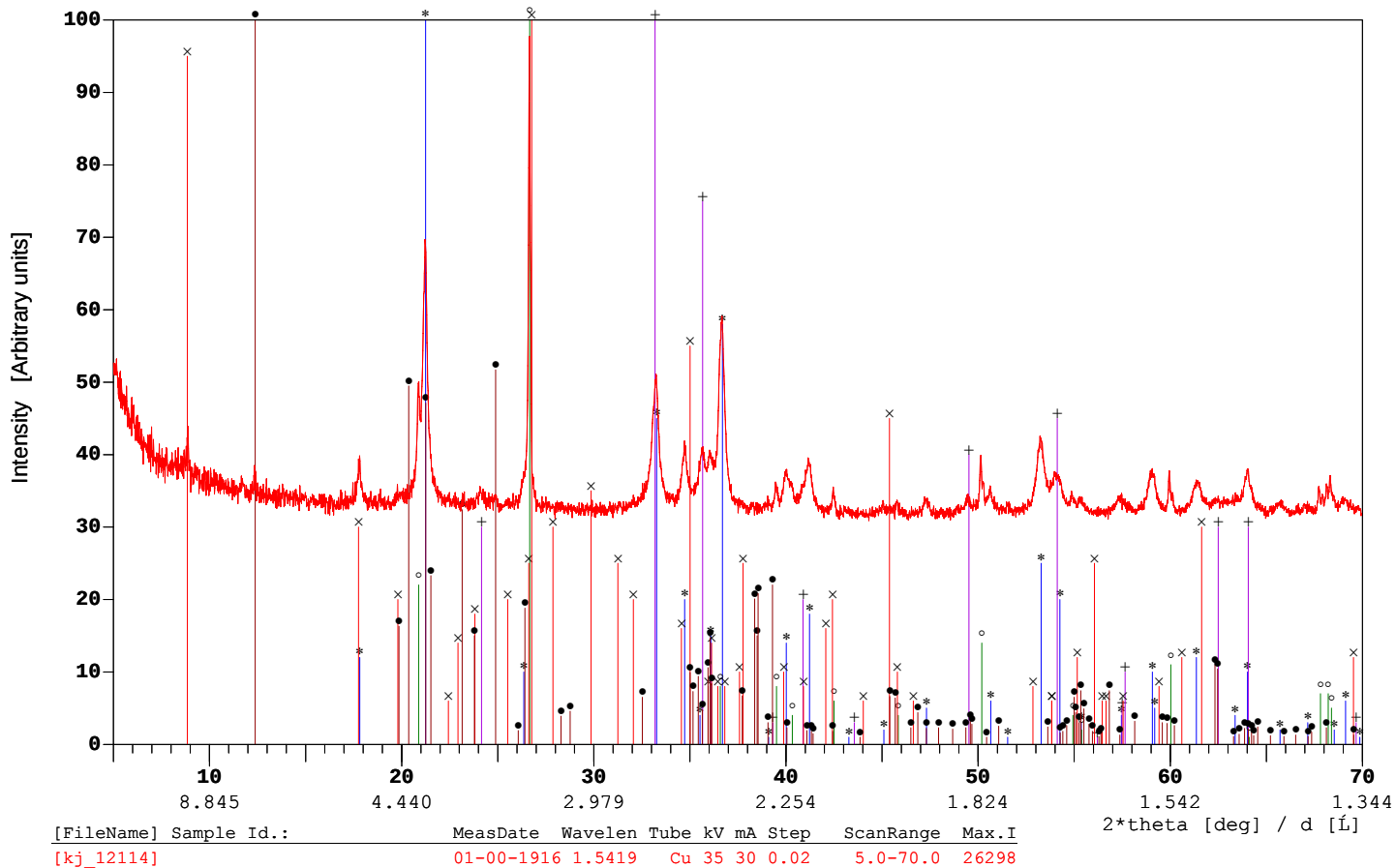
[KJ_12113]

	SUM	Goet	Hema	Quar	Musc	KaoT	Chem	
Phase%	100.00	86.00	5.00	5.00	1.00	3.00	Anal	Diff
Fe ₂ O ₃ %	82.28	77.28	5.00				65.00	-17.28
K ₂ O%	0.12				0.12		0.75	0.63
SiO ₂ %	6.85			5.00	0.45	1.40	17.30	10.45
Al ₂ O ₃ %	1.57				0.38	1.18	4.05	2.48
F%	0.02				0.02			
H ₂ O%	9.17	8.72			0.03	0.42		
LOI %	9.17	8.72	0.00	0.00	0.04	0.42	9.99	0.82

Orient.	[r]	1.00	1.00	1.00	0.50	0.70		
Shape	[exp]	1.50	1.50	1.50	1.50	1.50		
FWHM:	[0.10]	0.30	0.30	0.10	0.11	0.20		
xSize	[nm]	49	49	>1000	987	99		
pSize	[um]	3.0	3.0	5.0	3.0	1.0		
MAC	(CuKa)	197.7	218.9	34.5	42.3	29.8		
I/Ic		1.40	2.60	3.60	2.20	0.98		

Profile R = 0.03
 Chi square = 3.54
 Full Scale (obs) = 19914 counts
 Full Scale (calc) = 19914 counts
 2theta offset = 0.067 deg

XDB



Reference patterns:

*29-0713 Goet Goethite (revised) FeO(OH)
 +33-0664 Hema Hematite (revised) Fe2O3
 °33-1161 Quar Quartz SiO2
 x06-0263 Musc Muscovite 2M1 KAl2(Si3Al)O10(OH,F)2
 •79-1570 KaoT Kaolinite 1T Al2[Si2O5(OH)4]

[KJ_12114]

Phase%	SUM	Goet	Hema	Quar	Musc	KaoT	Chem	
	100.00	77.00	8.00	12.00	1.00	2.00	Anal	Diff
Fe ₂ O ₃ %	77.19	69.19	8.00				75.00	-2.19
K ₂ O%	0.12				0.12		0.40	0.28
SiO ₂ %	13.38			12.00	0.45	0.93	9.70	-3.68
Al ₂ O ₃ %	1.17				0.38	0.79	2.28	1.11
F%	0.02				0.02			
H ₂ O%	8.12	7.81			0.03	0.28		
LOI %	8.12	7.81	0.00	0.00	0.04	0.28	9.10	0.98

Orient.	[r]	1.00	1.00	1.00	0.50	0.70		
Shape	[exp]	1.50	1.50	1.50	1.50	1.50		
FWHM:	[0.10]	0.30	0.30	0.10	0.11	0.16		
xSize	[nm]	49	49	>1000	987	165		
pSize	[um]	3.0	3.0	5.0	3.0	1.0		
MAC	(CuKa)	197.7	218.9	34.5	42.3	29.8		
I/Ic		1.40	2.60	3.60	2.20	0.98		

Profile R = 0.03
 Chi square = 3.36
 Full Scale (obs) = 26298 counts
 Full Scale (calc) = 26298 counts
 2theta offset = 0.0 deg