

Whole Pattern Fitting and Rietveld Refinement

FILE: [A new.raw] B
SCAN: 5.0/89.9985/0.02046/19.1(sec), Cu(40kV,40mA), I(p)=2138, 07/29/24 09:46a
PROC: [WPF Control File]

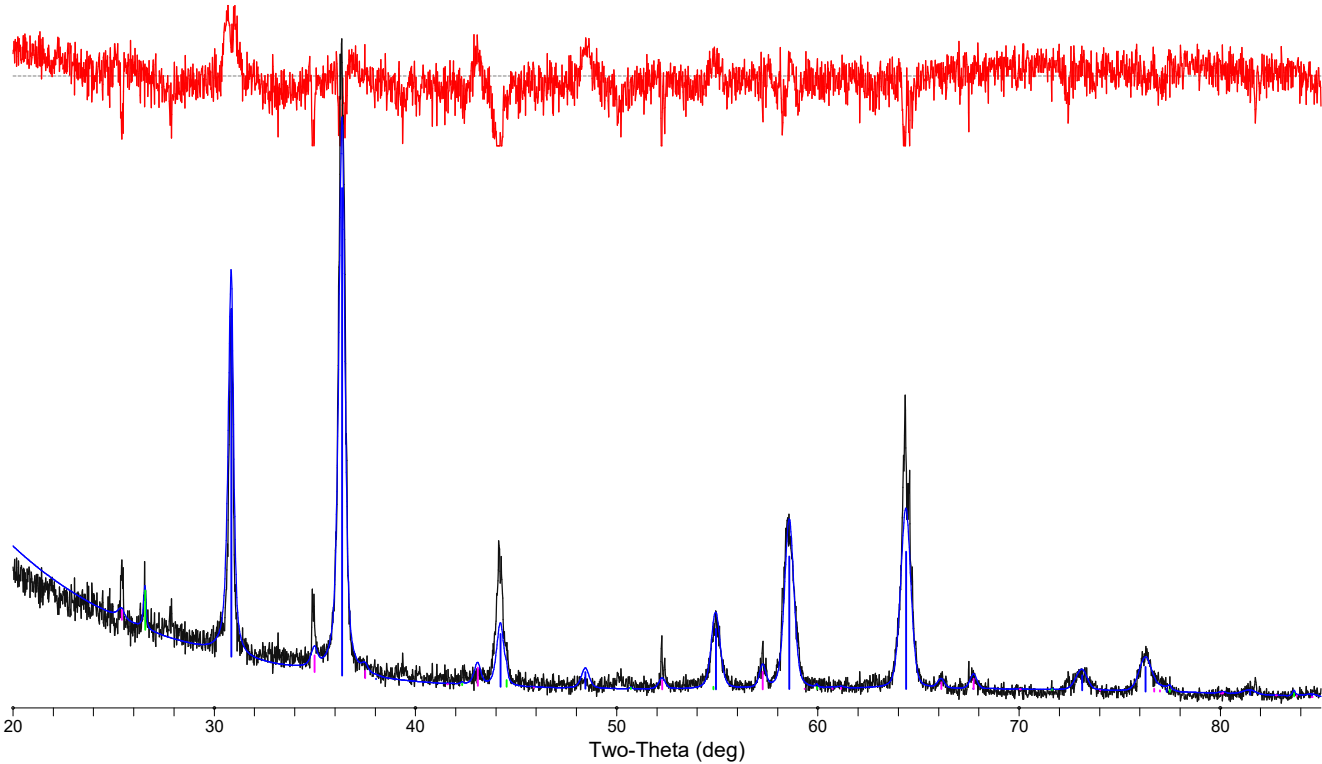
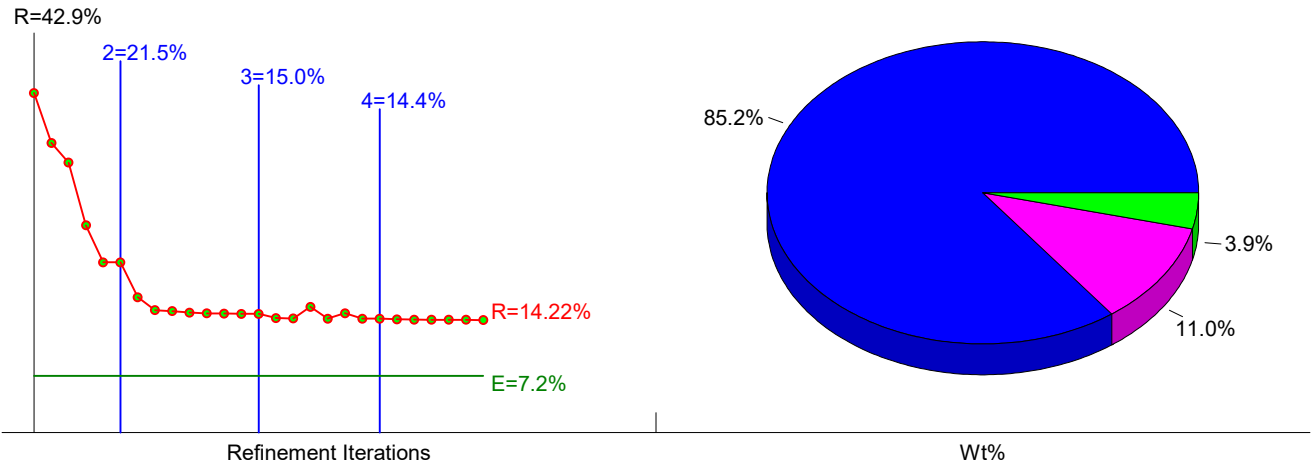
- ☒ Allow Negative Isotropic B
- ☒ Allow Negative Occupancy
- ☒ Apply Anomalous Scattering
- [Diffractometer LP] Two-Theta Range of Fit = 5.0 - 90.0(deg)
- ☒ Specimen Displacement - Cos(Theta) = -0.075701(0.013919)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Polynomial(2), Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (3)	Space Group	a	b	c	Alpha	Beta	Gamma
<div><div></div>Hercynite - Fe²⁺Al₂O₄</div>	Fd3̄m (227)	8.17237	8.17237	8.17237	90.000	90.000	90.000
<div><div></div>Corundum - Al₂O₃</div>	R3̄c (167)	4.78372	4.78372	13.00122	90.000	90.000	120.000
<div><div></div>Graphite - C</div>	P6 ₃ /mmc (194)	2.45977	2.45977	6.68703	90.000	90.000	120.000

Phase ID (3)	Source	I/Ic	Wt%	#L
<div><div></div>Hercynite - Fe²⁺Al₂O₄</div>	PDF#98-000-0242	3.33(0%)	85.2 (1.8)	19
<div><div></div>Corundum - Al₂O₃</div>	PDF#98-000-0174	1.04(0%)	11.0 (0.9)	26
<div><div></div>Graphite - C</div>	PDF#98-000-0231	2.46(0%)	3.9 (0.8)	11
XRF(Wt%): Fe=29.2%, Al=31.4%, O=35.6%, C=3.9%				

NOTE: Fitting Halted at Iteration 27(4): R=14.22% (E=7.2%, R/E=1.98, P=24, EPS=0.5)



Whole Pattern Fitting and Rietveld Refinement

FILE: [C.raw] C
SCAN: 5.0/89.9985/0.02046/19.1(sec), Cu(40kV,40mA), I(p)=2146, 07/26/24 07:50a
PROC: [WPF Control File]

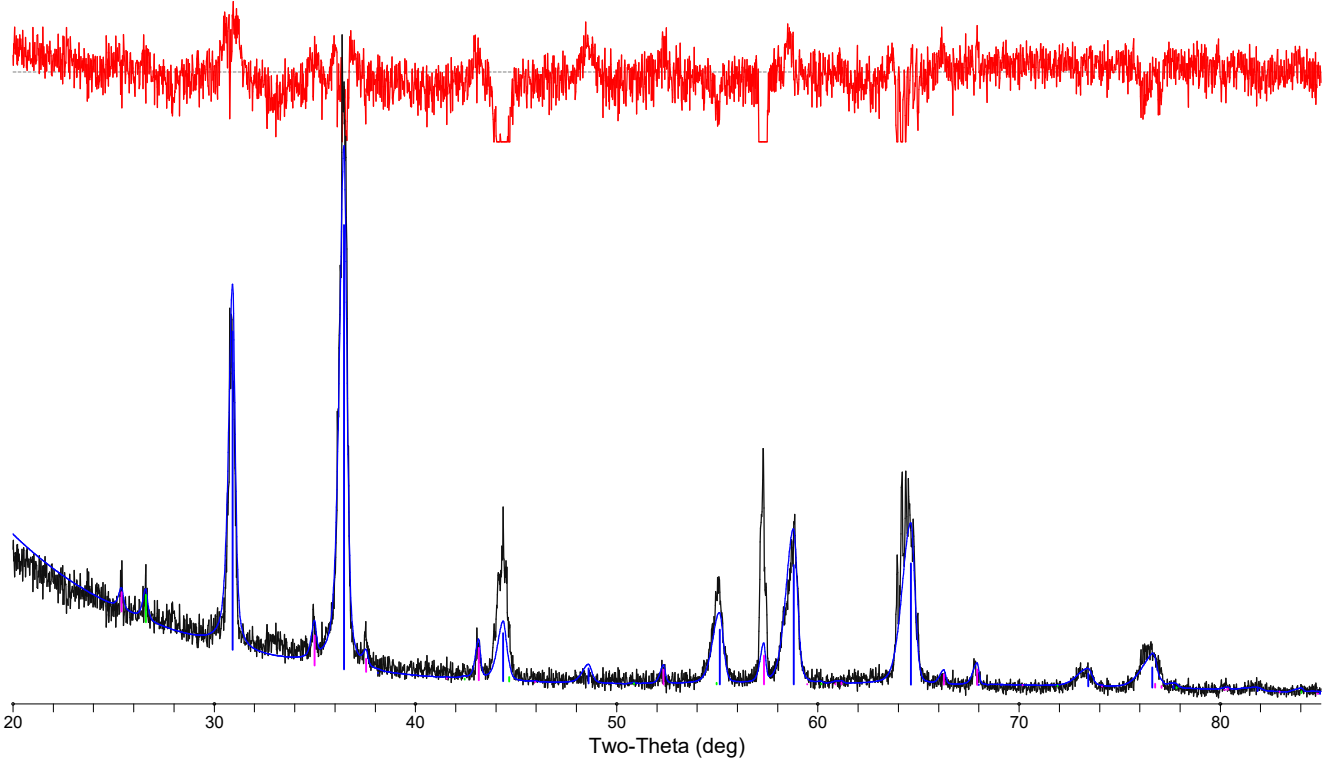
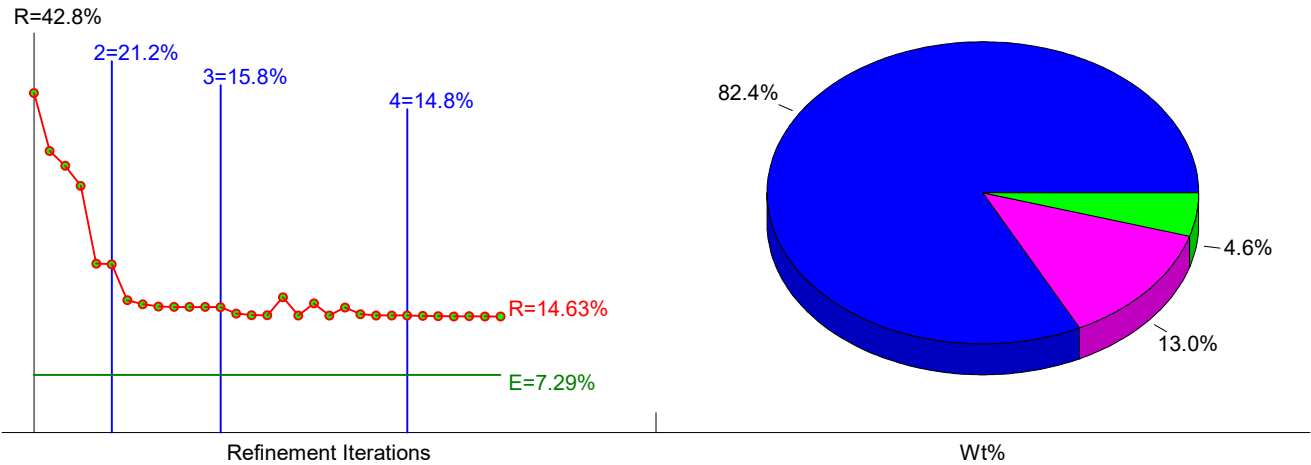
- ☒ Allow Negative Isotropic B
- ☒ Allow Negative Occupancy
- ☒ Apply Anomalous Scattering
- [Diffractometer LP] Two-Theta Range of Fit = 5.0 - 90.0(deg)
- ☒ Specimen Displacement - Cos(Theta) = -0.145253(0.016812)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Polynomial(2), Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (3)	Space Group	a	b	c	Alpha	Beta	Gamma
<div><div></div>Hercynite - Fe²⁺Al₂O₄</div>	Fd3̄m (227)	8.13787	8.13787	8.13787	90.000	90.000	90.000
<div><div></div>Corundum - Al₂O₃</div>	R3̄c (167)	4.76928	4.76928	12.98981	90.000	90.000	120.000
<div><div></div>Graphite - C</div>	P6 ₃ /mmc (194)	2.44979	2.44979	6.66147	90.000	90.000	120.000

Phase ID (3)	Source	I/Ic	Wt%	#L
<div><div></div>Hercynite - Fe²⁺Al₂O₄</div>	PDF#98-000-0242	3.35(0%)	82.4 (1.8)	18
<div><div></div>Corundum - Al₂O₃</div>	PDF#98-000-0174	1.04(0%)	13.0 (0.9)	26
<div><div></div>Graphite - C</div>	PDF#98-000-0231	2.48(0%)	4.6 (1.0)	11
XRF(Wt%): Fe=28.2%, Al=31.7%, O=35.5%, C=4.6%				

NOTE: Fitting Halted at Iteration 31(4): R=14.63% (E=7.29%, R/E=2.01, P=24, EPS=0.5)



PDF#98-000-0174: QM=Calculated; d=Calculated; I=(Unknown)												PDF Card	
Corundum													
Al ₂ O ₃													
Radiation=CuKa1				Lambda=1.5406				Filter=					
Calibration=				2T=25.579-117.864				I/Ic(RIR)=1.03					
Ref: Calculated from CSD#174 (MDI-500.csd) by Jade													
Hexagonal, R $\bar{3}$ c (167)											Z=6		
CELL: 4.7586 x 4.7586 x 12.9897 <90.0 x 90.0 x 120.0>											P.S=		
Density(c)=3.988		Density(m)=		Mwt=		Vol=254.7							
Ref: Ibid.													
NOTE: J Appl Cryst 20 (1987) 79, Thompson P, Cox D E, Hastings J B, See also PDF 10-173, 43-1484. [Corundum.csf]													
Strong Lines: 2.09/X 1.60/X 2.55/9 3.48/6 1.37/6 1.74/5 2.38/4 1.40/4													
42 Lines, Wavelength to Compute Theta = 1.54059Å(Cu), I%-Type = (Unknown)													
#	d(Å)	I(f)	(hkl)	2-Theta	Theta	1/(2d)	#	d(Å)	I(f)	(hkl)	2-Theta	Theta	1/(2d)
1	3.4797	57.3	(012)	25.579	12.789	0.1437	22	1.1386	0.2	(131)	85.148	42.574	0.4391
2	2.5507	91.9	(104)	35.155	17.578	0.1960	23	1.1257	3.6	(312)	86.360	43.180	0.4442
3	2.3793	40.0	(110)	37.779	18.890	0.2101	24	1.1240	2.6	(128)	86.517	43.258	0.4448
4	2.1650	0.6	(006)	41.685	20.843	0.2310	25	1.0988	7.5	(0,2,10)	89.015	44.507	0.4550
5	2.0852	100.0	(113)	43.358	21.679	0.2398	26	1.0825	1.8	(0,0,12)	90.731	45.366	0.4619
6	1.9641	1.7	(202)	46.182	23.091	0.2546	27	1.0782	8.8	(134)	91.198	45.599	0.4638
7	1.7399	47.8	(024)	52.557	26.279	0.2874	28	1.0462	0.2	(315)	94.830	47.415	0.4779
8	1.6013	95.8	(116)	57.508	28.754	0.3122	29	1.0426	17.3	(226)	95.261	47.630	0.4796
9	1.5465	2.0	(211)	59.746	29.873	0.3233	30	1.0175	2.1	(042)	98.403	49.202	0.4914
10	1.5147	3.4	(122)	61.135	30.568	0.3301	31	0.9976	12.9	(2,1,10)	101.095	50.547	0.5012
11	1.5107	6.8	(018)	61.314	30.657	0.3310	32	0.9853	0.2	(1,1,12)	102.849	51.425	0.5075
12	1.4044	36.7	(214)	66.525	33.263	0.3560	33	0.9820	2.5	(404)	103.328	51.664	0.5091
13	1.3737	56.2	(300)	68.215	34.108	0.3640	34	0.9732	0.1	(137)	104.655	52.327	0.5138
14	1.3359	1.0	(125)	70.425	35.212	0.3743	35	0.9429	0.4	(321)	109.552	54.776	0.5303
15	1.2753	1.4	(208)	74.313	37.156	0.3921	36	0.9410	0.3	(1,2,11)	109.885	54.942	0.5313
16	1.2389	16.0	(1,0,10)	76.890	38.445	0.4036	37	0.9356	0.2	(232)	110.840	55.420	0.5344
17	1.2340	8.1	(119)	77.250	38.625	0.4052	38	0.9346	3.7	(318)	111.008	55.504	0.5350
18	1.1930	0.6	(217)	80.430	40.215	0.4191	39	0.9180	2.8	(229)	114.091	57.045	0.5447
19	1.1897	6.3	(220)	80.706	40.353	0.4203	40	0.9078	12.8	(324)	116.114	58.057	0.5508
20	1.1599	0.8	(036)	83.227	41.614	0.4311	41	0.9052	4.5	(0,1,14)	116.638	58.319	0.5524
21	1.1471	5.0	(223)	84.364	42.182	0.4359	42	0.8993	7.3	(410)	117.864	58.932	0.5560

PDF#98-000-0242: QM=Calculated; d=Calculated; I=(Unknown)												PDF Card	
Hercynite Fe ²⁺ Al ₂ O ₄													
Radiation=CuKa1						Lambda=1.5406				Filter=			
Calibration=						2T=18.840-118.834				I/Ic(RIR)=3.32			
Ref: Calculated from CSD#242 (MDI-500.csd) by Jade													
Cubic, Fd $\bar{3}$ m (227)												Z=8	
CELL: 8.1517 x 8.1517 x 8.1517 <90.0 x 90.0 x 90.0>												P.S=	
Density(c)=4.399		Density(m)=		Mwt=		Vol=541.7							
Ref: Ibid.													
NOTE: Euro J Min 6 (1994) 39, Larsson, L.; O'Neill, H.S.C.; Annersten, H., See alos PDF 34-0192. [Hercynite.csf]													
Strong Lines: 2.46/X 2.88/6 1.44/5 1.57/4 1.66/2 1.06/1 2.04/1 0.94/1													
25 Lines, Wavelength to Compute Theta = 1.54059Å(Cu), I%-Type = (Unknown)													
#	d(Å)	I(f)	(hkl)	2-Theta	Theta	1/(2d)	#	d(Å)	I(f)	(hkl)	2-Theta	Theta	1/(2d)
1	4.7064	0.8	(111)	18.840	9.420	0.1062	14	1.2289	1.3	(622)	77.630	38.815	0.4069
2	2.8821	62.0	(220)	31.004	15.502	0.1735	15	1.1766	1.3	(444)	81.791	40.895	0.4250
3	2.4578	100.0	(311)	36.529	18.265	0.2034	16	1.1415	0.8	(711)	84.882	42.441	0.4380
4	2.3532	0.1	(222)	38.215	19.107	0.2125	17	1.0893	8.3	(642)	90.005	45.002	0.4590
5	2.0379	12.8	(400)	44.417	22.209	0.2453	18	1.0613	14.2	(553)	93.076	46.538	0.4711
6	1.8701	4.4	(331)	48.648	24.324	0.2674	19	1.0190	5.7	(800)	98.219	49.109	0.4907
7	1.6640	17.8	(422)	55.153	27.576	0.3005	20	0.9959	0.8	(733)	101.334	50.667	0.5021
8	1.5688	41.1	(511)	58.814	29.407	0.3187	21	0.9607	4.7	(822)	106.608	53.304	0.5205
9	1.4410	46.0	(440)	64.626	32.313	0.3470	22	0.9413	10.7	(751)	109.840	54.920	0.5312
10	1.3779	0.2	(531)	67.979	33.989	0.3629	23	0.9351	1.1	(662)	110.932	55.466	0.5347
11	1.3586	0.1	(442)	69.078	34.539	0.3680	24	0.9114	1.6	(840)	115.384	57.692	0.5486
12	1.2889	5.7	(620)	73.402	36.701	0.3879	25	0.8948	0.6	(753)	118.834	59.417	0.5588
13	1.2431	9.6	(533)	76.580	38.290	0.4022							

