

MO6-Evaluation report (MO6)

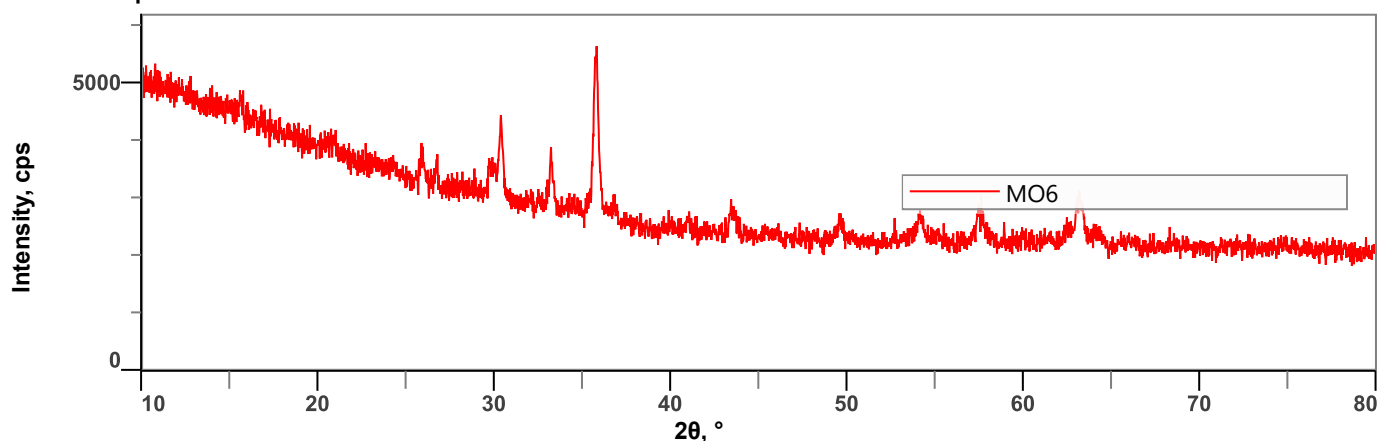
General information

Name	Value	Name	Value
Analysis date	2023-12-04 11:18:26	Measurement star...	2023-12-04 10:52:16
Analyst	Administrator	Operator	Administrator
Sample name		Comment	
Measured data na...	E:\Data from XRD\SERVICE DATA\2023\...	Memo	

Measurement Conditions

Name	Value	Name	Value
X-Ray generator	40 kV, 40 mA	Scan mode	1D(scan)
Incident primary	Standard	Scan speed/Durati...	5.00 °/min
Goniometer	Standard Goniometer	Step width	0.02 °
Attachment	Standard	Scan axis	$\theta/2\theta$
Filter	K β filter 1D for Cu	Scan range	10 ~ 80 °
Selection slit	PB	Incident slit box	1.000mm
Diffacted beam...	None	Length-limiting slit	10 mm
Detector	D/teX Ultra 250 (H)	Receiving slit box...	Open
Optics attribute	PB	Receiving slit box...	Open

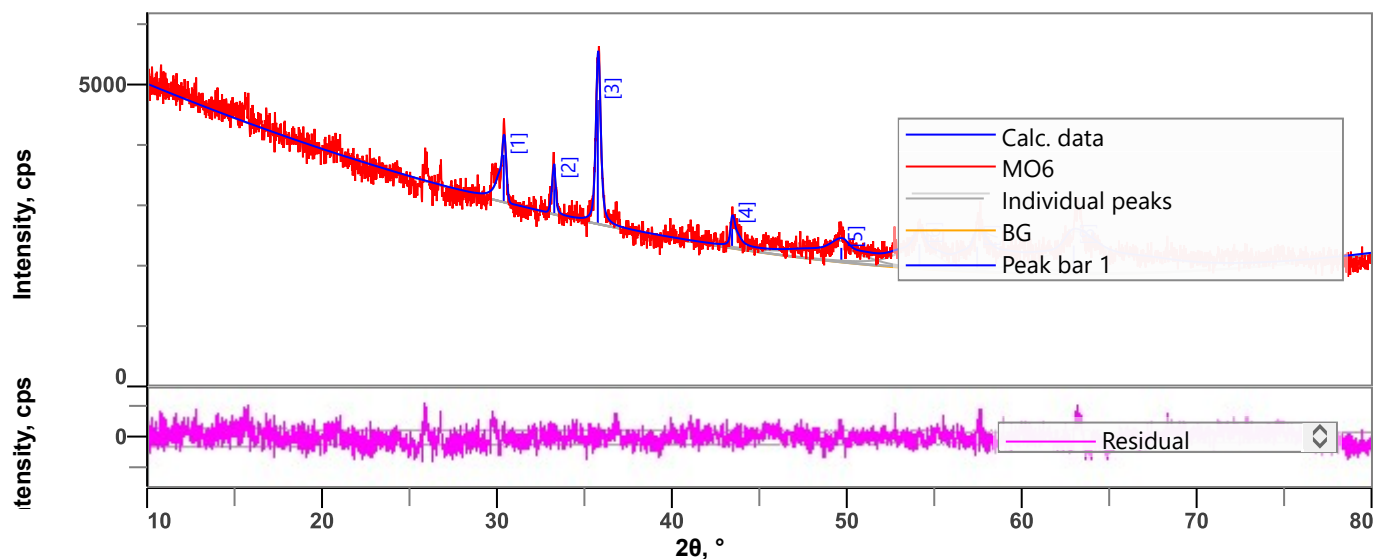
Measured profile view



Peak profiling conditions

Name	Value	Name	Value	Name	Value
Peak search...	Second derivative met...	σ cut	3.00		
Profile fitting	Run completed	Peak shape	Split pseudo-Voigt	Fitting condition	Auto(Refine background)

Peak Profile View



Peak list

No.	2θ, °	d, Å	Height, cps	FWHM, °	Int. I., cps°	Int. W., °
1	30.36(3)	2.941(2)	787(24)	0.31(4)	409(29)	0.52(5)
2	33.25(3)	2.692(2)	590(20)	0.22(4)	156(21)	0.26(4)
3	35.737(16)	2.5105(11)	2054(57)	0.287(13)	796(24)	0.39(2)
4	43.40(5)	2.083(2)	407(16)	0.27(9)	205(24)	0.50(8)
5	49.64(14)	1.835(5)	240(9)	1.9(3)	994(135)	4.1(7)
6	54.10(8)	1.694(2)	413(16)	1.22(17)	1070(138)	2.6(4)
7	57.40(8)	1.604(2)	424(17)	1.5(2)	1316(200)	3.1(6)
8	62.92(5)	1.4760(10)	477(19)	3.4(2)	3419(279)	7.2(9)

No.	2θ, °	Asymmetry	Decay(ηL/mL)	Decay(ηH/mH)	Size, Å	Phase Name
1	30.36(3)	1.4(5)	1.5(2)	0.0(5)	278(32)	Magnetite: 2 2 0
2	33.25(3)	3(3)	0.0(6)	1.2(10)	398(67)	Unknown: 0 0 0
3	35.737(16)	1.0(2)	0.60(17)	0.71(17)	304(14)	Magnetite: 3 1 1
4	43.40(5)	0.6(6)	0.8(9)	1.5(4)	327(105)	Magnetite: 4 0 0
5	49.64(14)	1.6(8)	1.55(17)	1.5(2)	47(7)	
6	54.10(8)	1.3(6)	1.55(14)	1.55(18)	77(10)	Magnetite: 4 2 2
7	57.40(8)	0.5(2)	1.55(19)	1.55(12)	65(9)	Magnetite: 5 1 1
8	62.92(5)	0.50(13)	1.55(14)	1.55(5)	28.9(18)	Magnetite: 4 4 0

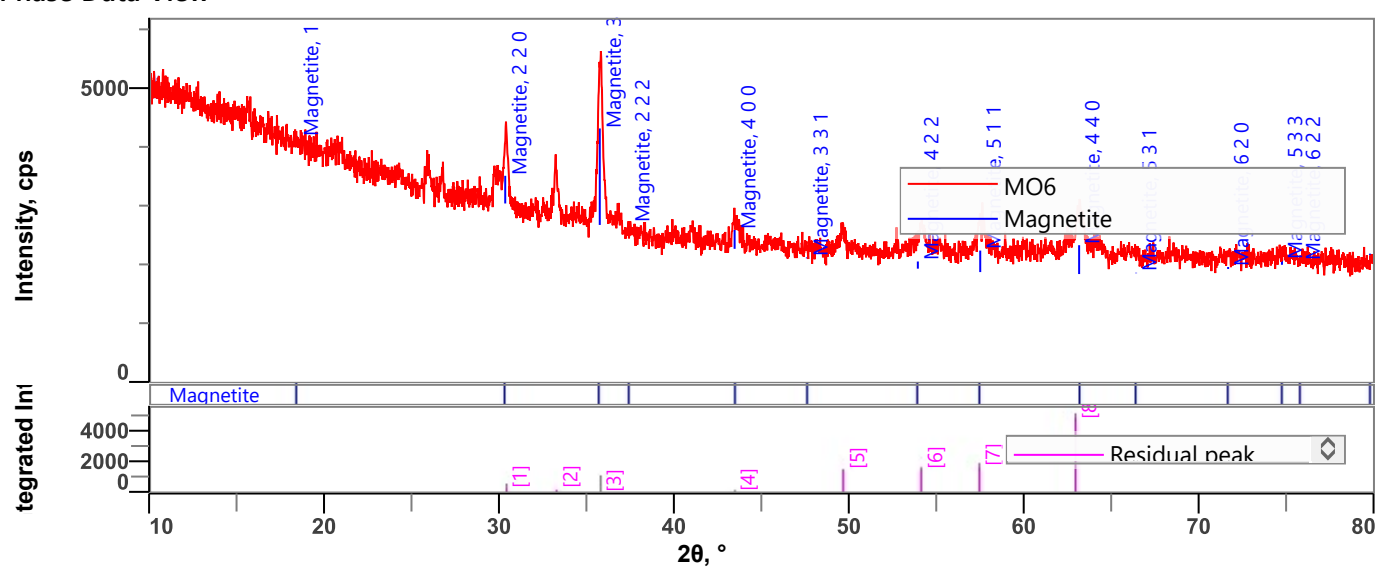
No.	2θ, °	Chemical Formula	Card No	Norm. I.	Profile Type	Distributi...
1	30.36(3)	Fe ₃ O ₄	01-075-0449	11.97	Split pseudo-Voigt	-
2	33.25(3)			4.57	Split pseudo-Voigt	-
3	35.737(16)	Fe ₃ O ₄	01-075-0449	23.27	Split pseudo-Voigt	-
4	43.40(5)	Fe ₃ O ₄	01-075-0449	6.00	Split pseudo-Voigt	-
5	49.64(14)			29.07	Split pseudo-Voigt	-
6	54.10(8)	Fe ₃ O ₄	01-075-0449	31.31	Split pseudo-Voigt	-
7	57.40(8)	Fe ₃ O ₄	01-075-0449	38.51	Split pseudo-Voigt	-
8	62.92(5)	Fe ₃ O ₄	01-075-0449	100.00	Split pseudo-Voigt	-

No.	2 θ , °	Degree of Orientati...	Ring Factor	β Cluster
1	30.36(3)	-	-	-
2	33.25(3)	-	-	-
3	35.737(16)	-	-	-
4	43.40(5)	-	-	-
5	49.64(14)	-	-	-
6	54.10(8)	-	-	-
7	57.40(8)	-	-	-
8	62.92(5)	-	-	-

Qualitative analysis results

Phase name	Formula	Figure of merit	Phase reg. detail	Space Group	DB Card Number
Magnetite	Fe ₃ O ₄	0.924	S/M(PDF-2 Releas...	227 : Fd-3m:2	01-075-0449

Phase Data View



Lattice parameters

Phase name	a, Å	b, Å	c, Å	α , °	β , °	γ , °
Magnetite	8.32687	8.32687	8.32687	90.000	90.000	90.000

d-I List**Magnetite**

No.	2θ , °	d, Å	h k l	Norm. I.
1	18.44018	4.80752	1 1 1	6.10
2	30.33599	2.94399	2 2 0	28.10
3	35.73441	2.51065	3 1 1	100.00
4	37.38084	2.40376	2 2 2	7.50
5	43.43482	2.08172	4 0 0	20.20
6	47.56050	1.91032	3 3 1	1.10
7	53.89723	1.69972	4 2 2	8.10
8	57.45989	1.60251	5 1 1	24.80
9	57.45989	1.60251	3 3 3	0.00
10	63.10776	1.47200	4 4 0	34.40
11	66.36128	1.40750	5 3 1	0.60
12	67.42744	1.38781	4 4 2	0.00
13	71.61550	1.31659	6 2 0	2.50
14	74.68968	1.26984	5 3 3	6.30
15	75.70399	1.25532	6 2 2	2.50
16	79.71930	1.20188	4 4 4	2.00