01-075-6876 Apr 28, 2021 12:51 PM (wongng)

PDF Card

Status: Alternate **Quality Mark:** Star **Environment:** Ambient
Temperature of Data Collection: 298.0 K (Assigned by ICDD editor) **Chemical Formula:** Mn O
Empirical Formula: Mn O **Weight %:** Mn77.45 O22.55 **Atomic %:** Mn50.00 O50.00
Compound Name: Manganese Oxide **Mineral Name:** Manganosite, syn
Entry Date: 09/01/2008 **Modification Date:** 09/01/2020 **Modifications:** Update

Experimental

Radiation: CuKα1 (1.5406 Å) **d-Spacing:** Calculated **Intensity:** Calculated - Peak

Physical

Crystal System: Cubic **SPGR:** Fm-3m (225)

Author's Unit Cell

a: 4.446(1) Å **Volume:** 87.88 Å^3 **Z:** 4.00
MolVol: 21.97

Calculated Density: 5.361 g/cm^3 **Structural Density:** 5.36 g/cm^3
SS/FOM: F(10) = 999.9(0.0000, 10) **R-factor:** 0.0102 **I/Ic:** 5.13 **I/Ic - CW ND:** 1.12

Crystal

ICDD Calculated Parameters

Space Group: Fm-3m (225) **Molecular Wt:** 70.94 g/mol

Crystal Data

a: 4.446 Å **b:** 4.446 Å **c:** 4.446 Å
α: 90.00° **β:** 90.00° **γ:** 90.00°
Volume: 87.88 Å^3 **Z:** 4.00 **a/b:** 1.000
c/b: 1.000

Reduced Cell

a: 3.144 Å **b:** 3.144 Å **c:** 3.144 Å
α: 60.00° **β:** 60.00° **γ:** 60.00°
Volume: 21.97 Å^3

Structure

Atomic parameters are cross-referenced from PDF entry 04-005-4310

AC Space Group: Fm-3m (225)

AC Unit Cell

a: 4.446(1) Å	**b:** 4.446(1) Å	**c:** 4.446(1) Å
α: 90°	**β:** 90°	**γ:** 90°

Space Group Symmetry Operators:

Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator
1	x,y,z	13	x,-y,-z	25	-x,y,-z	37	-x,-y,z
2	-x,-y,-z	14	-x,y,z	26	x,-y,z	38	x,y,-z
3	z,x,y	15	z,-x,-y	27	-z,x,-y	39	-z,-x,y
4	-z,-x,-y	16	-z,x,y	28	z,-x,y	40	z,x,-y
5	y,z,x	17	y,-z,-x	29	-y,z,-x	41	-y,-z,x
6	-y,-z,-x	18	-y,z,x	30	y,-z,x	42	y,z,-x
7	x,z,y	19	x,-z,-y	31	-x,z,-y	43	-x,-z,y
8	-x,-z,-y	20	-x,z,y	32	x,-z,y	44	x,z,-y
9	y,x,z	21	y,-x,-z	33	-y,x,-z	45	-y,-x,z
10	-y,-x,-z	22	-y,x,z	34	y,-x,z	46	y,x,-z
11	z,y,x	23	z,-y,-x	35	-z,y,-x	47	-z,-y,x
12	-z,-y,-x	24	-z,y,x	36	z,-y,x	48	z,y,-x

Atomic Displacement Parameter Type: B

Atomic Coordinates:

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	Biso	AET
Mn	1	4a	m-3m	0.0	0.0	0.0	1.0	0.617	6-a
O	2	4b	m-3m	0.5	0.5	0.5	1.0	0.72	6-a

Crystal (Symmetry Allowed): Centrosymmetric **AC Space Group:** Fm-3m (225)

Classifications

Subfiles: Common Phase, Forensic, Inorganic, Metal & Alloy, Mineral Related (Mineral, Synthetic)

Mineral Classification: Halite (group), oxide (subgroup) **Pearson Symbol:** cF8.00

Prototype Structure (Formula Order): Na Cl **Prototype Structure (Alpha Order):** Cl Na

LPF Prototype Structure (Formula Order): Na Cl,cF8,225

LPF Prototype Structure (Alpha Order): Cl Na,cF8,225 **ANX:** AX

Wyckoff Sequence: b a (FM-3M)

Cross-references

Cross-Ref PDF #'s: 00-001-1206 (Deleted), 00-002-1158 (Deleted), 00-003-1145 (Deleted), 00-006-0592 (Deleted), 00-007-0230 (Primary), 01-071-4748 (Alternate), 01-072-1533 (Alternate), 01-075-0257 (Alternate), 01-075-0625 (Alternate), 01-075-0626 (Alternate), 01-077-2363 (Alternate), 01-089-2804 (Alternate), 04-001-7707 (Alternate), 04-002-5597 (Alternate), 04-002-5617 (Alternate), 04-002-8159 (Alternate), 04-002-8344 (Alternate), 04-003-5838 (Alternate), 04-003-7148 (Alternate), 04-004-8991 (Alternate), 04-005-4310 (Primary), 04-005-4397 (Alternate), 04-005-4473 (Alternate), 04-005-9717 (Alternate), 04-005-9791 (Alternate), 04-006-0700 (Alternate), 04-006-1771 (Alternate), 04-006-1784 (Alternate), 04-006-3696 (Alternate), 04-006-3703 (Alternate), 04-006-5363 (Alternate), 04-007-3408 (Alternate), 04-007-3620 (Alternate), 04-007-8200 (Alternate), 04-007-8377 (Alternate), 04-008-0277 (Alternate), 04-008-2747 (Alternate), 04-008-6796 (Alternate), 04-011-7332 (Alternate), 04-013-0265 (Alternate), 04-015-2351 (Alternate)

References

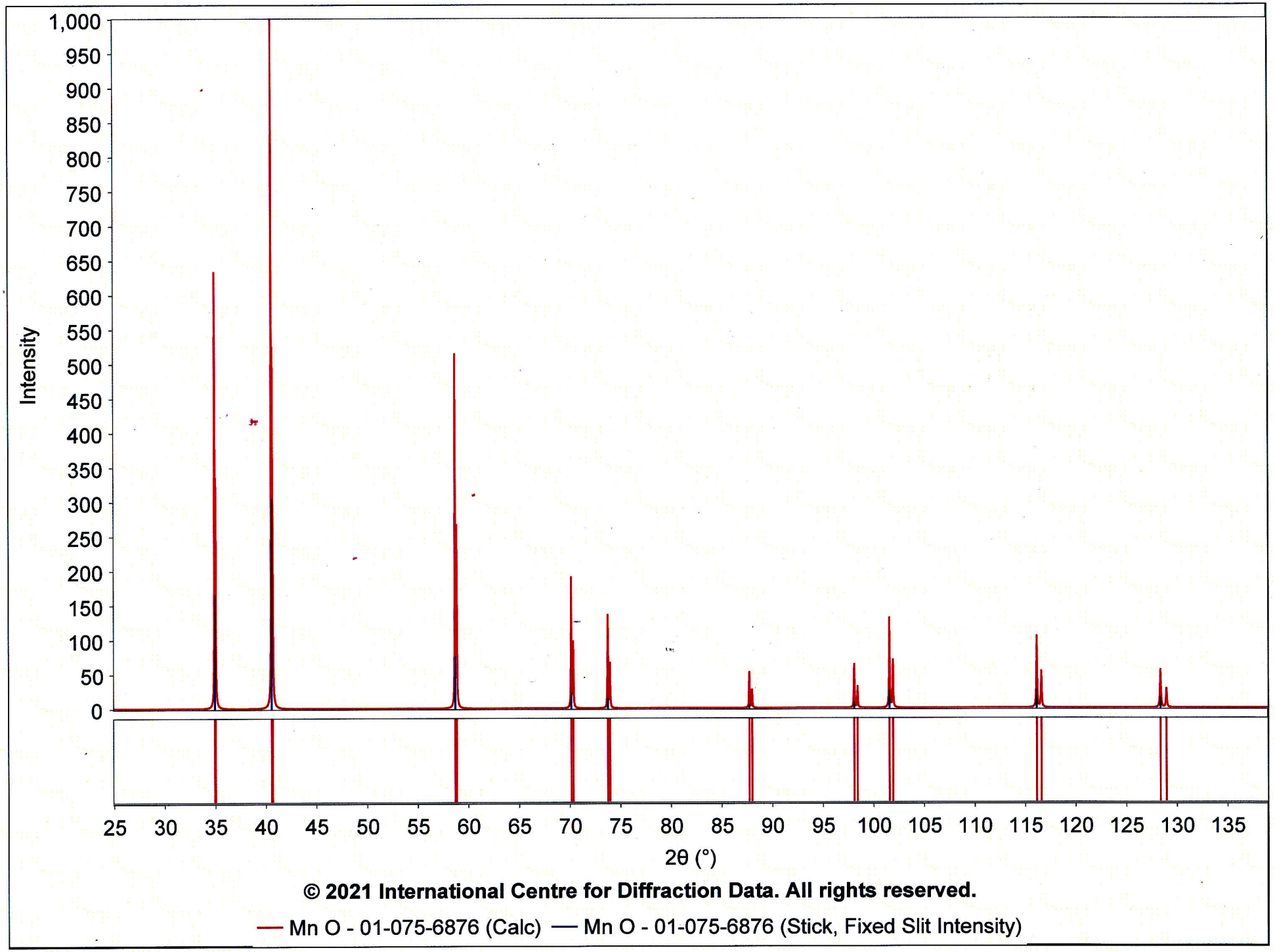
Type	DOI	Reference
Primary Reference		Calculated from ICSD using POWD-12++.
Crystal Structure		Crystal Structure Source: LPF.
Structure	10.2183/pjab.55.43	Sasaki, S., Fujino, K., Takeuchi, Y. "X-ray determination of electron-density distributions in oxides, Mg O, Mn O, Co O, and Ni O, and atomic scattering factors of their constituent atoms". Proc. Jpn. Acad. 1979, 55, 43.

Comments

Database Comments: ANX: AX. Analysis: Mn1 O1. Formula from original source: Mn O. ICSD Collection Code: 9864. Wyckoff Sequence: b a (FM-3M). Unit Cell Data Source: Single Crystal.

d-spacings (10) - Mn O - 01-075-6876 (Stick, Fixed Slit Intensity) - X-ray (Cu Kα1 1.54056

2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*
34.925	**2.566900**	622	1	1	1		87.738	1.111500	51	4	0	0	
40.547	**2.223000**	1000	2	0	0		98.084	1.019980	60	3	3	1	
58.685	**1.571900**	499	2	2	0		101.575	0.994156	130	4	2	0	
70.145	1.340520	182	3	1	1		116.154	0.907536	101	4	2	2	
73.763	1.283450	129	2	2	2		128.381	0.855633	52	5	1	1	


1,000
950
900
850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
Intensity
25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135
2θ (°)
© 2021 International Centre for Diffraction Data. All rights reserved.
Mn O - 01-075-6876 (Calc)
Mn O - 01-075-6876 (Stick, Fixed Slit Intensity)