

# PDF Card No.: 00-030-0794 Quality:O

Sub-File Name: Inorganic, Alloy&Metal, Cement&Hydration Product, Corrosion, Pharmaceutical, Supercond...

Formula: Mg O

Name: Magnesium Oxide

I/Ic (RIR)= ---

Crystal System: Cubic

Space Group: Fd-3m(227)

Dmeas:

Cell Parameters: a= 8.1200

b= 8.1200

c= 8.1200

Alpha= 90.000

Beta= 90.000

Gamma= 90.000

Volume= 535.387

Z= 20

Reference: Freund. Ber. Dtsch. Keram. Ges.47(1970)739.

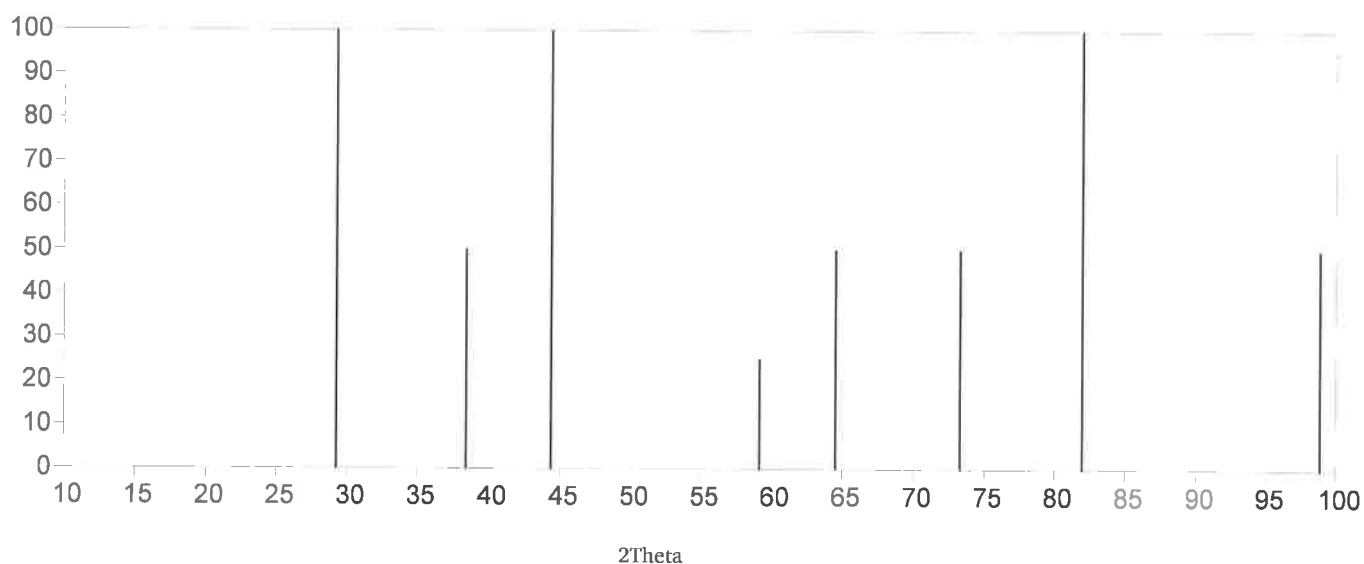
Radiation: CuK $\alpha$

Wavelength= 1.54180

2Theta range: 29.26 - 98.87

Database comments: Reason O Quality Was Assigned: O assigned because of mixture. Sample Preparation: Synthetic "Mg (O H )<sup>2</sup>", dehydrated for 36 hours at 400 C, gives mixed periclase and spinel type pattern; these are the reflections which index on a spinel cell. Unit Cell Data Source: Powder Diffraction.

Relative Intensity



No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	29.26	3.050	100.0										
2	38.44	2.340	50.0	2	2	2							
3	44.37	2.040	100.0	4	0	0							
4	59.18	1.560	25.0	5	1	1							
5	64.53	1.443	50.0	4	4	0							
6	73.33	1.290	50.0	6	2	0							
7	82.01	1.174	100.0	4	4	4							
8	98.87	1.014	50.0	8	0	0							

Note: 2theta are calculated with wavelength = 1.54056

# PDF Card No.: 00-019-0771 Quality:O

Sub-File Name: Inorganic, Alloy&Metal, Corrosion, Superconducting Material

Formula: Mg O<sub>2</sub>

Name: Magnesium Oxide

I/I<sub>c</sub> (RIR) = ---

Crystal System: Unknown

Space Group: (0)

D<sub>meas</sub>:

Cell Parameters: a=

b=

c=

Alpha=

Beta=

Gamma=

Volume=

Z=

Reference: Allamagny. Rev. Chim. Miner.2(1965)645.

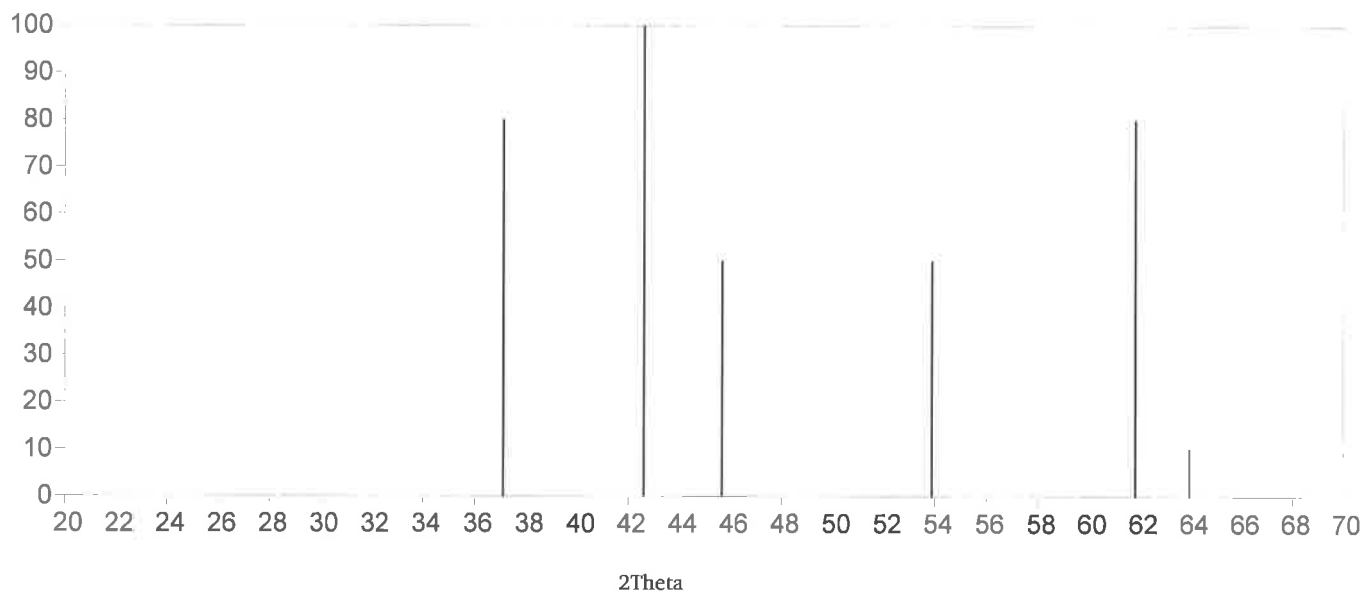
Radiation: CuK $\alpha$ 1

Wavelength= 1.54050

2Theta range: 37.12 - 63.93

Database comments: Reason O Quality Was Assigned: O assigned because of poor fit of measured "d" values to hkl indices. Unit Cell Data Source: Powder Diffraction.

Relative Intensity



No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	37.12	2.420	80.0										
2	42.61	2.120	100.0										
3	45.67	1.985	50.0										
4	53.89	1.700	50.0										
5	61.84	1.499	80.0										
6	63.93	1.455	10.0										

Note: 2theta are calculated with wavelength = 1.54056

# PDF Card No.: 01-076-1363 Quality:B

Sub-File Name: Inorganic, Alloy&Metal, Corrosion, ICSD Pattern

Formula: Mg O2

Name: magnesium peroxide

I/Ic (RIR)= 2.10

Crystal System: Cubic Space Group: Pa-3(205) Dmeas: 3.180

Cell Parameters: a= 4.8390 b= 4.8390 c= 4.8390

Alpha= 90.000 Beta= 90.000 Gamma= 90.000

Volume= 113.310 Z= 4

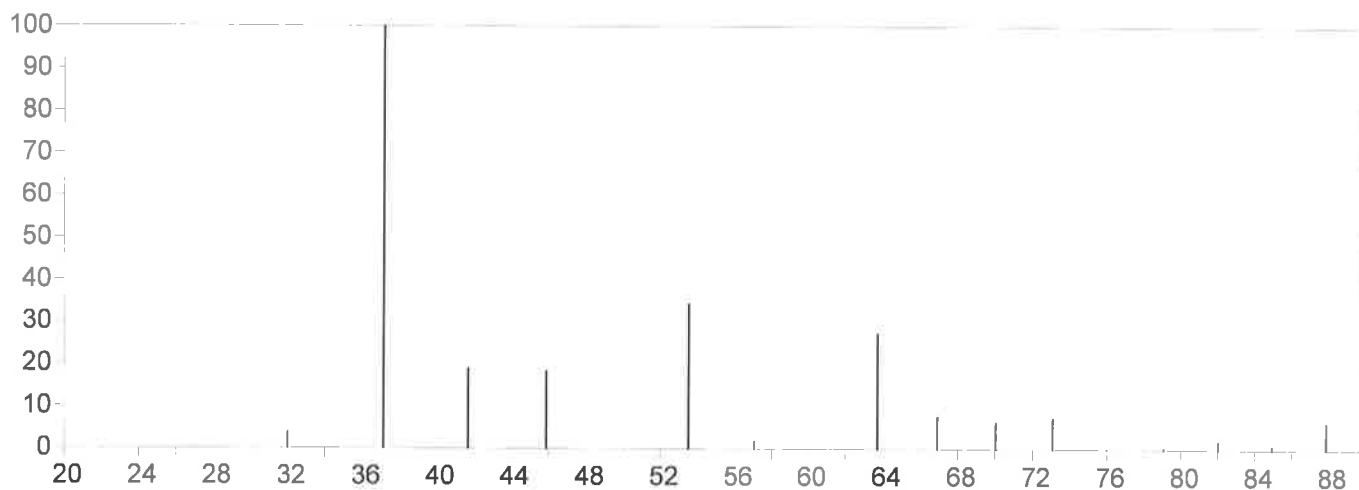
Reference: Vannerberg, N.G. Ark. Kemi14(1959)99.

Radiation: CuK $\alpha$ 1 Wavelength= 1.54060

2Theta range: 32.01 - 87.87

Database comments: Additional Patterns: See PDF 00-019-0771. ANX: AX2. ICSD Collection Code: 35479. Other Cell: Cell from Acta Chem. Scand., Ser. A, 33 617-620 (1979): 4.8441, xyz (O)=.0886. Test from ICSD: At least one TF missing. Calc. density unusual but tolerable. Significant Warning: ICSD Warning: The coordinates are those given in the paper but the atomic distances do not agree with those calculated during testing. The coordinates are probably correct. Wyckoff Sequence: c b (PA3-). Unit Cell Data Source: Powder

Relative Intensity



2Theta

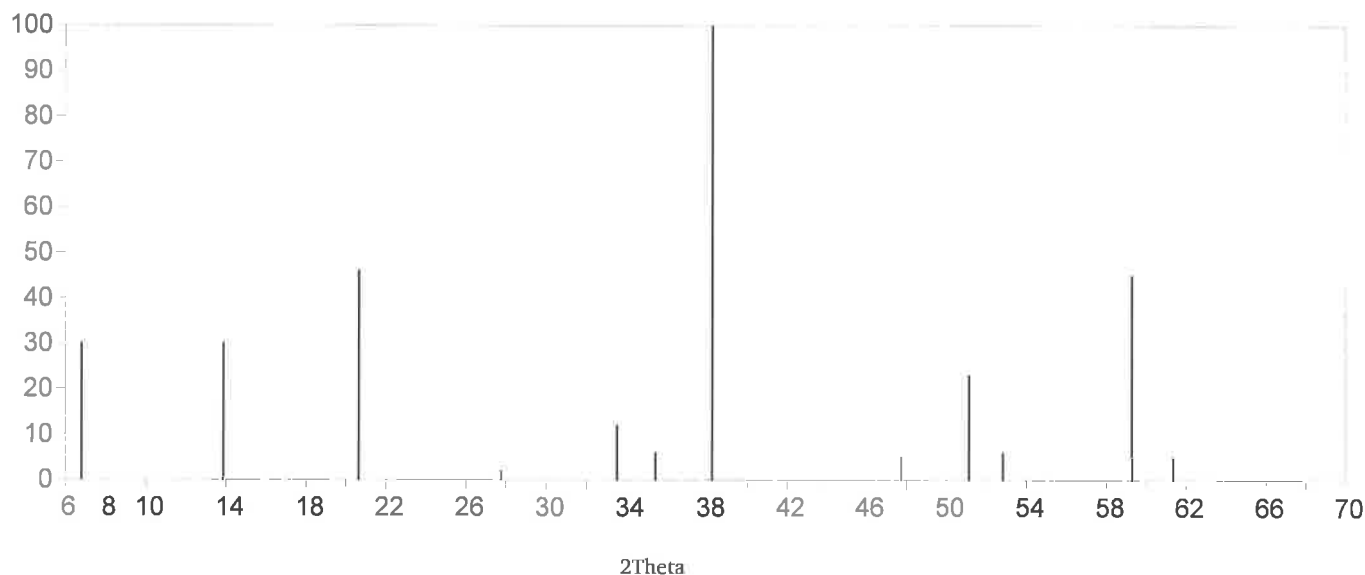
No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	32.01	2.794	3.7	1	1	1							
2	37.13	2.420	100.0	2	0	0							
3	41.70	2.164	18.9	2	1	0							
4	45.90	1.976	18.4	2	1	1							
5	53.52	1.711	34.3	2	2	0							
6	57.05	1.613	1.8	2	2	1							
7	63.73	1.459	27.3	3	1	1							
8	66.93	1.397	7.6	2	2	2							
9	70.05	1.342	6.2	0	2	3							
10	73.11	1.293	7.3	3	2	1							
11	79.10	1.210	0.4	4	0	0							
12	82.04	1.174	1.8	3	2	2							
13	84.96	1.141	0.8	4	1	1							
14	87.87	1.110	6.3	3	3	1							

Note: 2theta are calculated with wavelength = 1.54056

# PDF Card No.: 00-047-0237 Quality:B

Sub-File Name:	Inorganic, Corrosion				
Formula:	( Mg0.88 Al0.12 ( O H )2 )2 ( ( C O3 )0.12 ( H2 O )0.64 )				
Name:	Magnesium Aluminum Carbonate Hydroxide Hydrate				I/Ic (RIR)= ---
Crystal System:	Trigonal		Space Group: R-3m(166)		Dmeas:
Cell Parameters:	a=	3.1080	b=	3.1080	c= 38.3000
	Alpha=	90.000	Beta=	90.000	Gamma= 120.000
	Volume=	320.399	Z=	--	
Reference:	Grey, I., Ragozzini, R. J. Solid State Chem.94(1991)244.				
Radiation:	CuKá		Wavelength= 1.54180		
2Theta range:	6.79 - 61.34				
Database comments:	Sample Preparation: Prepared by adding "Mg O" to an aqueous solution containing "Na O H", "Na2 C O3" and dissolved "Al" foil. Structures: Isostructural with coalingite. Unit Cell Data Source: Powder Diffraction.				

Relative Intensity



No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	6.79	13.000	30.0	0	0	3							
2	13.85	6.390	30.0	0	0	6							
3	20.64	4.300	46.0	0	0	9							
4	27.77	3.210	2.0	0	0	12							
5	33.54	2.670	12.0	0	1	2							
6	35.45	2.530	6.0	0	1	5							
7	38.27	2.350	100.0	0	1	8							
8	47.75	1.903	5.0	0	1	14							
9	51.16	1.784	23.0	1	0	16							
10	52.85	1.731	6.0	0	1	17							
11	59.30	1.557	45.0	1	1	0							
12	61.34	1.510	5.0	1	1	6							

Note: 2theta are calculated with wavelength = 1.54056

# PDF Card No.: 00-014-0525 Quality:B

Sub-File Name: Inorganic, Mineral, Corrosion

Formula:  $\text{Mg}_6\text{Al}_2\text{C}_3\text{O}_{16}(\text{OH})_4\cdot 4\text{H}_2\text{O}$

Name: Manasseite

I/Ic (RIR) = ---

Crystal System: Hexagonal Space Group: P63/mmc(194) Dmeas: 2.050

Cell Parameters: a= 6.1200 b= 6.1200 c= 15.3240

Alpha= 90.000 Beta= 90.000 Gamma= 120.000

Volume= 497.056 Z= 1

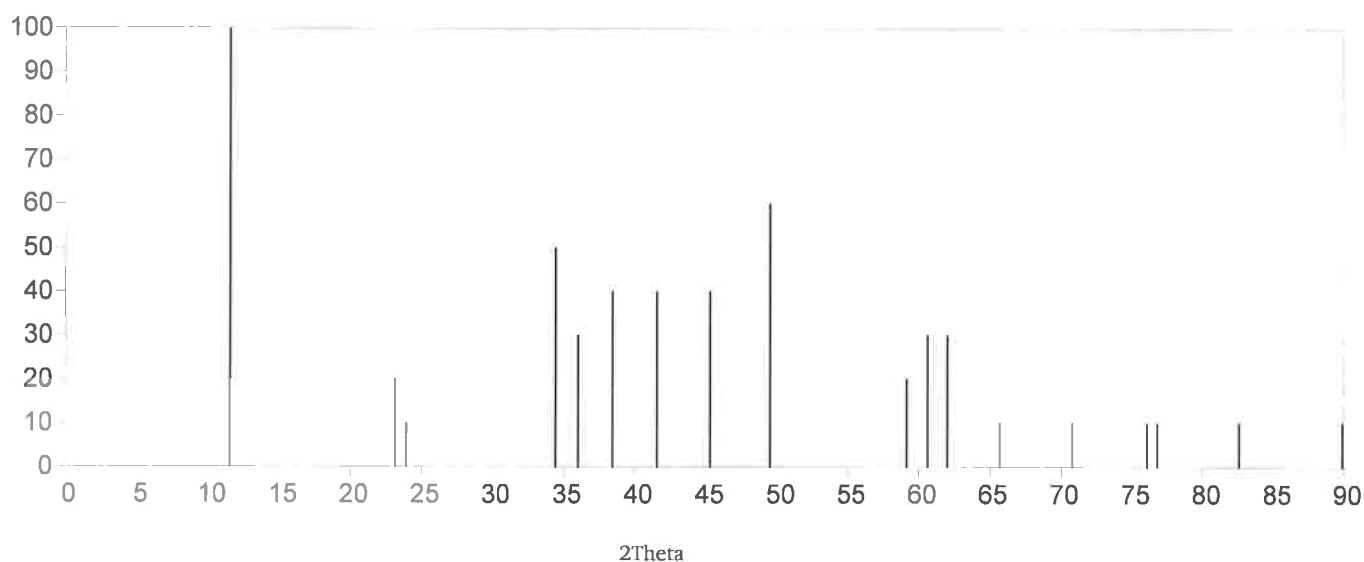
Reference: Neumann, Bergstol, Mineral. Museum, Oslo, Norway. Private Communication().

Radiation: FeK $\alpha$  Wavelength= 1.93730

2Theta range: 11.53 - 89.93

Database comments: Color: White, light black. Footnotes for D-spacings and Intensities: 1 Corresponds with published diagram of Newmann, Sellevall, Arh. Norsk Videnskap. Akad. Oslo, 1 (1955).  
Sample Source or Locality: Specimen from Dypingdal, Snarum, Norway. Unit Cell Data  
Source: Powder Diffraction.

Relative Intensity



No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	11.53	7.670	100.0	0	0	2							
2	23.20	3.830	20.0	0	0	4							
3	23.97	3.710	10.0	1	0	3							
4	34.47	2.600	50.0	2	0	1							
5	36.04	2.490	30.0	2	0	2							
6	38.44	2.340	40.0	2	0	3							
7	41.58	2.170	40.0	2	0	4							
8	45.30	2.000	40.0	2	1	0							
9	49.50	1.840	60.0	2	0	6							
10	59.18	1.560	20.0	2	0	8							
11	60.68	1.525	30.0	2	2	0							
12	62.07	1.494	30.0	2	2	2							
13	65.70	1.420	10.0	2	2	4							
14	70.78	1.330	10.0	2	0	10							
15	76.08	1.250	10.0	4	0	4							
16	76.81	1.240	10.0	1	0	12							
17	82.61	1.167	10.0	3	1	8							
18	89.93	1.090	10.0	4	0	8							

Note: 2theta are calculated with wavelength = 1.54056

# PDF Card No.: 01-073-1959 Quality:I

Sub-File Name: Inorganic, Corrosion, ICSD Pattern

Formula: Mg Al2 O4

Name: magnesium dialuminium oxide

I/Ic (RIR) = 1.87

Crystal System: Cubic Space Group: Fd-3m(227) Dmeas:

Cell Parameters: a= 8.0500 b= 8.0500 c= 8.0500

Alpha= 90.000 Beta= 90.000 Gamma= 90.000

Volume= 521.660 Z= 8

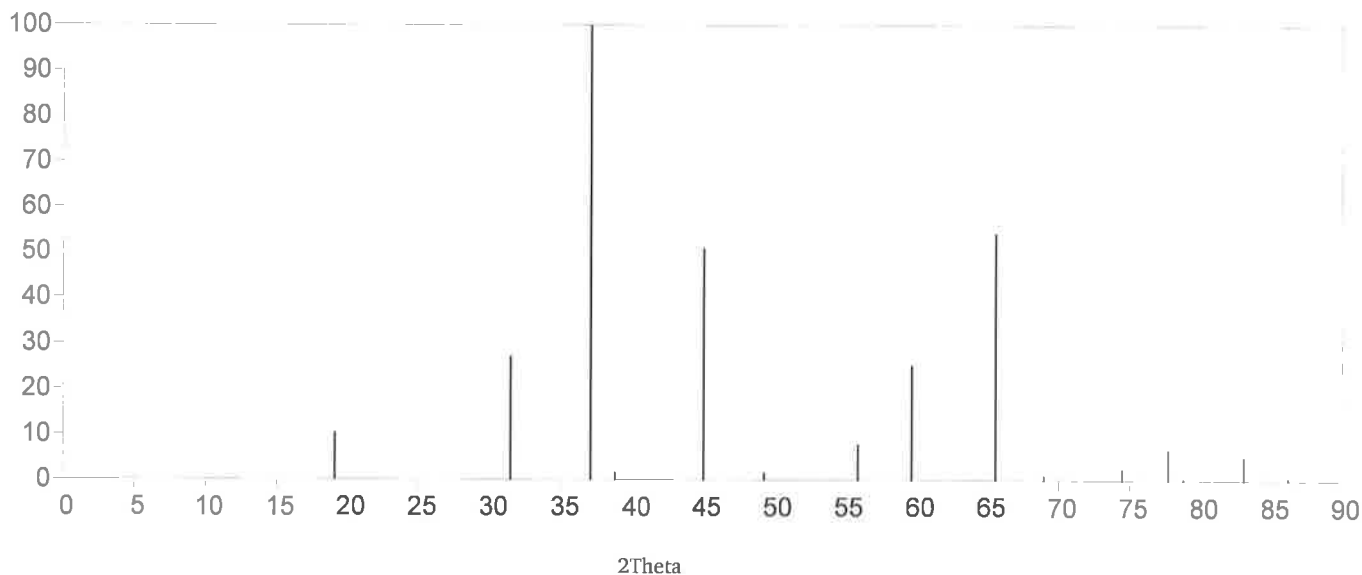
Reference: Passerini, L. Gazz. Chim. Ital.60(1930)389.

Radiation: CuK $\alpha$ 1 Wavelength= 1.54060

2Theta range: 19.08 - 86.21

Database comments: ANX: AB2X4. ICSD Collection Code: 24492. Test from ICSD: No R value given. At least one TF missing. Minor Warning: No R value given in the paper. Wyckoff Sequence: e d a (FD3-MS).

Relative Intensity



No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	19.08	4.648	10.2	1	1	1							
2	31.41	2.846	27.0	2	2	0							
3	37.01	2.427	100.0	3	1	1							
4	38.72	2.324	1.5	2	2	2							
5	45.01	2.013	50.8	4	0	0							
6	49.30	1.847	1.5	3	3	1							
7	55.91	1.643	7.7	4	2	2							
8	59.63	1.549	25.1	5	1	1							
9	65.54	1.423	54.1	4	4	0							
10	68.96	1.361	0.9	5	3	1							
11	74.48	1.273	2.4	6	2	0							
12	77.73	1.228	6.6	5	3	3							
13	78.80	1.214	0.2	6	2	2							
14	83.05	1.162	5.0	4	4	4							
15	86.21	1.127	0.4	7	1	1							

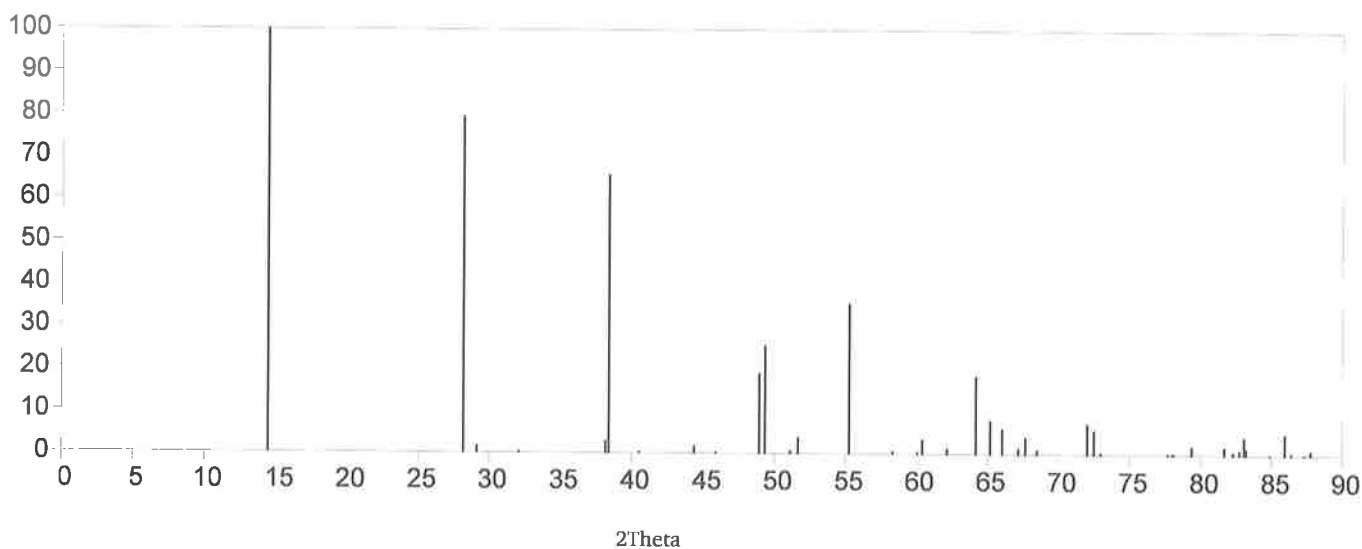
Note: 2theta are calculated with wavelength = 1.54056

# PDF Card No.: 01-074-1895 Quality:I

Sub-File Name:	Inorganic, Mineral, Common Phase, Corrosion, Forensic, ICSD Pattern				
Formula:	Al O ( O H )				
Name:	Bohmite, syn				I/Ic (RIR)= 1.37
Crystal System:	Orthorhombic		Space Group:	Cmcm(63)	Dmeas: 2.970
Cell Parameters:	a=	2.8590	b=	12.2400	c= 3.6910
	Alpha=	90.000	Beta=	90.000	Gamma= 90.000
	Volume=	129.163	Z=	4	
Reference:	Reichertz, P.P., Yost, W.J. J. Chem. Phys.14(1946)495.				
Radiation:	CuKá1		Wavelength= 1.54060		
2Theta range:	14.46 - 87.75				

Database comments: Additional Patterns: See PDF 01-083-2384 and PDF 00-021-1307. ANX: AX2. ICSD Collection Code: 27865. Calculated Pattern Original Remarks: ATOM H 1 +1 4.00 Atoms not located in unit cell. Test from ICSD: Calc. density unusual but tolerable. At least one TF missing. No R value given. Minor Warning: No R value given in the paper. Incomplete determination of H atom positions in the structure. Wyckoff Sequence: c3 (CMCM). Unit Cell Data Source: Powder Diffraction.

Relative Intensity



No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	14.46	6.120	100.0	0	2	0	21	66.05	1.413	5.9	0	8	1
2	28.21	3.161	79.4	0	2	1	22	67.19	1.392	1.3	2	2	0
3	29.16	3.060	1.5	0	4	0	23	67.69	1.383	3.9	1	7	1
4	32.12	2.784	0.3	1	1	0	24	68.50	1.369	1.0	0	6	2
5	38.17	2.356	2.8	0	4	1	25	72.04	1.310	7.1	1	5	2
6	38.41	2.341	65.6	1	3	0	26	72.51	1.302	5.6	2	2	1
7	40.55	2.223	0.2	1	1	1	27	72.99	1.295	0.4	2	4	0
8	44.37	2.040	1.6	0	6	0	28	77.69	1.228	0.2	1	9	0
9	45.86	1.977	0.2	1	3	1	29	78.00	1.224	0.2	0	10	0
10	48.94	1.859	18.8	1	5	0	30	78.14	1.222	0.1	2	4	1
11	49.34	1.845	25.3	0	0	2	31	79.38	1.206	1.9	0	2	3
12	51.12	1.785	0.6	0	6	1	32	81.68	1.178	1.8	0	8	2
13	51.69	1.767	3.7	0	2	2	33	82.29	1.171	0.6	2	6	0
14	55.27	1.661	35.4	1	5	1	34	82.75	1.165	1.0	1	9	1
15	58.34	1.580	0.5	0	4	2	35	83.06	1.162	4.1	0	10	1
16	60.10	1.538	0.4	1	1	2	36	83.21	1.160	1.4	1	7	2
17	60.46	1.530	3.3	0	8	0	37	84.87	1.142	0.1	0	4	3
18	62.18	1.492	1.3	1	7	0	38	85.94	1.130	4.9	2	0	2
19	64.21	1.449	18.3	1	3	2	39	86.39	1.125	0.4	1	1	3
20	65.21	1.429	7.8	2	0	0	40	87.30	1.116	0.1	2	6	1

Note: 2theta are calculated with wavelength = 1.54056

# PDF Card No.: 00-047-0254 Quality:I

Sub-File Name: Inorganic, Corrosion

Formula: Mg Al<sub>2</sub> O<sub>4</sub>

Name: Magnesium Aluminum Oxide

I/Ic (RIR) = ---

Crystal System: Orthorhombic

Space Group: Pnam(62)

Dmeas:

Cell Parameters: a= 8.6310

b= 9.9690

c= 2.7890

Alpha= 90.000

Beta= 90.000

Gamma= 90.000

Volume= 239.972

Z= 4

Reference: Irifune, T., Fujino, K., Ohtani, E. Nature (London)349(1991)409.

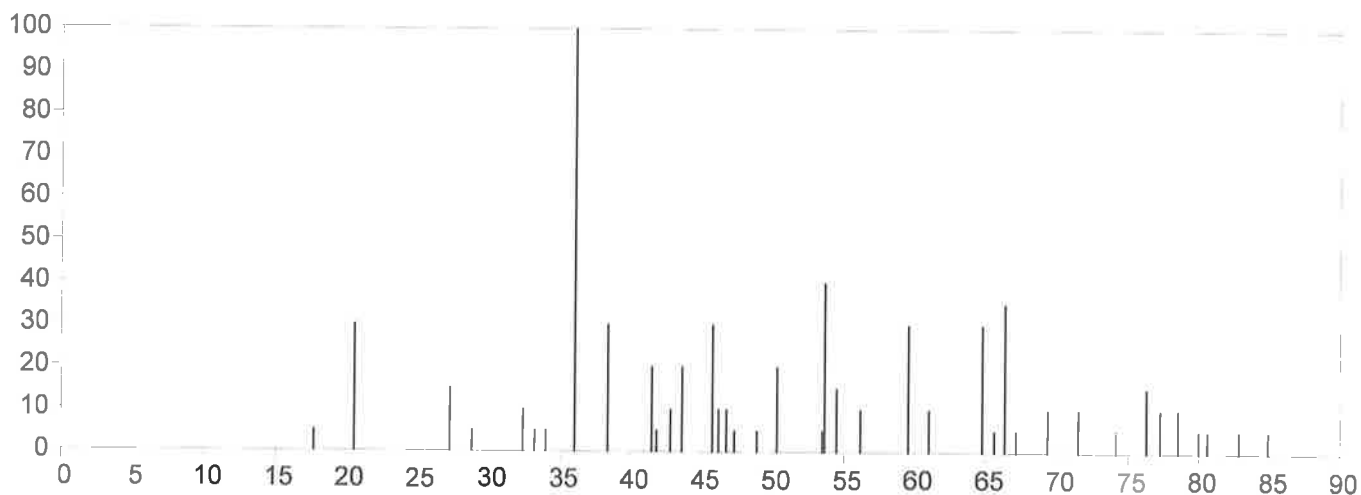
Radiation: CuK $\alpha$

Wavelength= 1.54180

2Theta range: 17.72 - 84.91

Database comments: Sample Preparation: A powder was formed from the single crystals. A new phase was observed after a pressure of 26 GPa and temperature of 1500 C were applied and the sample quenched to ambient pressure and temperature. Sample Source or Locality: Single-crystal spinel ("Mg Al<sub>2</sub> O<sub>4</sub>"), from Union Carbide Co., USA, was used as starting material. Structures: Similar to calcium ferrite, ("Ca Fe<sub>2</sub> O<sub>4</sub>"). Unit Cell Data Source: Powder Diffraction.

Relative Intensity



2Theta

No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	17.72	5.000	5.0	0	2	0	21	53.67	1.706	40.0	4	0	1
2	20.59	4.310	30.0	2	0	0	22	54.52	1.682	15.0	4	1	1
3	27.33	3.260	15.0	2	2	0	23	56.21	1.635	10.0	3	5	0
4	28.86	3.091	5.0	1	3	0	24	59.58	1.550	30.0	2	6	0
5	32.40	2.761	10.0	3	1	0	25	61.00	1.518	10.0	4	3	1
6	33.23	2.694	5.0	0	1	1	26	64.75	1.439	30.0	6	0	0
7	33.99	2.635	5.0	2	3	0	27	65.60	1.422	5.0	6	1	0
8	36.03	2.491	100.0	3	2	0	28	66.34	1.408	35.0	1	6	1
9	38.35	2.345	30.0	2	0	1	29	67.12	1.393	5.0	0	0	2
10	41.46	2.176	20.0	3	3	0	30	69.36	1.354	10.0	2	6	1
11	41.80	2.159	5.0	4	0	0	31	71.52	1.318	10.0	4	6	0
12	42.78	2.112	10.0	4	1	0	32	74.18	1.277	5.0	3	6	1
13	43.60	2.074	20.0	1	3	1	33	76.31	1.247	15.0	6	4	0
14	45.76	1.981	30.0	4	2	0	34	77.28	1.234	10.0	1	8	0
15	46.21	1.963	10.0	3	1	1	35	78.53	1.217	10.0	3	2	2
16	46.76	1.941	10.0	1	5	0	36	80.00	1.198	5.0	7	2	0
17	47.33	1.919	5.0	2	3	1	37	80.61	1.191	5.0	4	6	1
18	48.93	1.860	5.0	3	2	1	38	82.83	1.164	5.0	4	1	2
19	50.31	1.812	20.0	1	4	1	39	84.91	1.141	5.0	4	2	2
20	53.51	1.711	5.0	3	3	1							

Note: 2theta are calculated with wavelength = 1.54056



# PDF Card No.: 01-071-6335 Quality:S

Sub-File Name: Inorganic, Mineral, ICSD Pattern

Formula: Mg Al<sub>2</sub> O<sub>4</sub>

Name: magnesium dialuminum oxide, spinel HP

I/Ic (RIR) = 1.69

Crystal System: Cubic Space Group: Fd-3m(227) Dmeas:

Cell Parameters: a= 8.0340 b= 8.0340 c= 8.0340

Alpha= 90.000 Beta= 90.000 Gamma= 90.000

Volume= 518.556 Z= 8

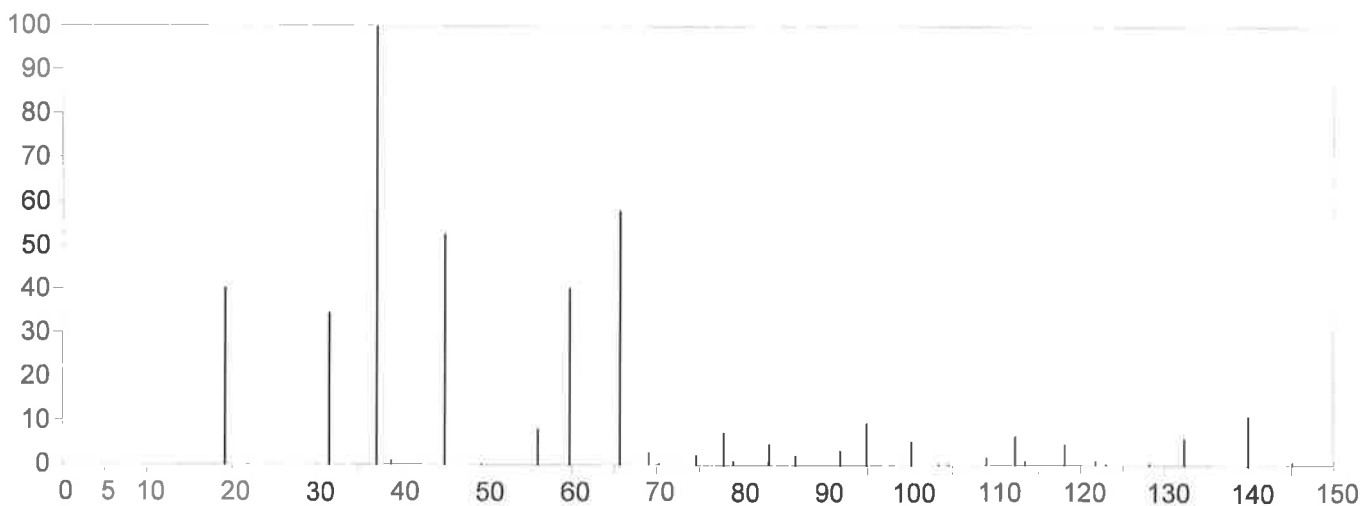
Reference: Finger, L.W., Hazen, R.M., Hofmeister, A.M. Phys. Chem. Miner.13(1986)215.

Radiation: CuK $\alpha$ 1 Wavelength= 1.54060

2Theta range: 19.12 - 145.10

Database comments: ANX: AB2X4. ICSD Collection Code: 77587. Pressure of Datacollection: 4000 MPa.  
Calculated Pattern Original Remarks: First SG setting assumed origin at -3m. ICSD entry Z77587 is filename FIZZ77587. Sample Source or Locality: Specimen from SE Asia. Wyckoff Sequence: e d a (FD3-MZ).

Relative Intensity



2Theta

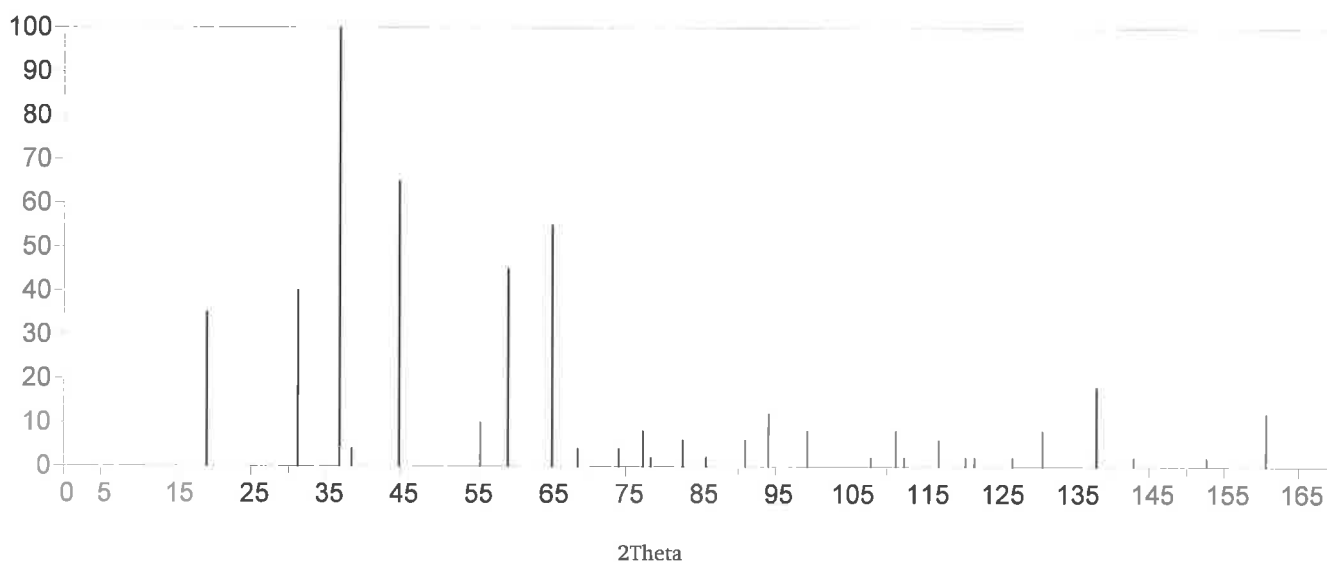
No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	19.12	4.638	40.2	1	1	1	21	104.49	0.974	0.1	6	4	4
2	31.47	2.840	34.5	2	2	0	22	108.89	0.947	1.5	8	2	2
3	37.08	2.422	100.0	3	1	1	23	112.26	0.928	6.5	7	5	1
4	38.80	2.319	0.9	2	2	2	24	113.41	0.922	0.7	6	6	2
5	45.10	2.009	52.5	4	0	0	25	118.09	0.898	4.6	8	4	0
6	49.41	1.843	0.1	3	3	1	26	121.73	0.882	0.9	9	1	1
7	56.03	1.640	8.1	4	2	2	27	122.98	0.877	0.1	8	4	2
8	59.76	1.546	40.2	5	1	1	28	128.16	0.856	0.3	6	6	4
9	65.69	1.420	57.8	4	4	0	29	132.30	0.842	6.0	9	3	1
10	69.11	1.358	2.6	5	3	1	30	139.90	0.820	11.2	8	4	4
11	70.24	1.339	0.1	4	4	2	31	145.10	0.807	0.5	9	3	3
12	74.66	1.270	2.2	6	2	0							
13	77.91	1.225	7.3	5	3	3							
14	78.99	1.211	0.8	6	2	2							
15	83.25	1.160	4.7	4	4	4							
16	86.42	1.125	2.1	7	1	1							
17	91.69	1.074	3.2	6	4	2							
18	94.86	1.046	9.5	7	3	1							
19	100.17	1.004	5.3	8	0	0							
20	103.40	0.982	0.1	7	3	3							

Note: 2theta are calculated with wavelength = 1.54056

# PDF Card No.: 00-021-1152 Quality:S

Sub-File Name:	Inorganic, Mineral, Common Phase, Corrosion, Educational Pattern, Forensic, NBS Pattern				
Formula:	Mg Al2 O4				
Name:	Spinel, syn			I/Ic (RIR)= 1.70	
Crystal System:	Cubic	Space Group: Fd-3m(227)		Dmeas:	
Cell Parameters:	a= 8.0831	b= 8.0831	c= 8.0831		
	Alpha= 90.000	Beta= 90.000	Gamma= 90.000		
	Volume= 528.122	Z= 8			
Reference:	Natl. Bur. Stand. (U.S.) Monogr. 259(1971)25.				
Radiation:	CuKα1	Wavelength= 1.54050			
2Theta range:	19.03 - 160.65				
Database comments:	Color: Colorless. Sample Preparation: Shell used a carbon electrode furnace and removed an excess of MgO with hot HCl after crushing. Sample Source or Locality: The sample was furnished by H.R. Shell, Bureau of Mines, College Park, Maryland, USA. Temperature of Data Collection: Pattern taken at 298 K. Unit Cell Data Source: Powder Diffraction.				

Relative Intensity



No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	19.03	4.660	35.0	1	1	1	21	116.92	0.904	6.0	8	4	0
2	31.27	2.858	40.0	2	2	0	22	120.50	0.887	2.0	9	1	1
3	36.85	2.437	100.0	3	1	1	23	121.70	0.882	2.0	8	4	2
4	38.52	2.335	4.0	2	2	2	24	126.76	0.862	2.0	6	6	4
5	44.83	2.020	65.0	4	0	0	25	130.73	0.847	8.0	9	3	1
6	55.66	1.650	10.0	4	2	2	26	138.07	0.825	18.0	8	4	4
7	59.37	1.555	45.0	5	1	1	27	142.98	0.812	2.0	7	7	1
8	65.24	1.429	55.0	4	4	0	28	152.68	0.793	2.0	10	2	0
9	68.64	1.366	4.0	5	3	1	29	160.65	0.781	12.0	9	5	1
10	74.13	1.278	4.0	6	2	0							
11	77.32	1.233	8.0	5	3	3							
12	78.40	1.219	2.0	6	2	2							
13	82.64	1.167	6.0	4	4	4							
14	85.76	1.132	2.0	5	5	1							
15	90.97	1.080	6.0	6	4	2							
16	94.10	1.052	12.0	7	3	1							
17	99.34	1.010	8.0	8	0	0							
18	107.90	0.953	2.0	6	6	0							
19	111.23	0.933	8.0	7	5	1							
20	112.32	0.927	2.0	6	6	2							

Note: 2theta are calculated with wavelength = 1.54056