APPENDIX A.

JCPDS

Pattern : 74-816 **Radiation =** 1.540600 **Quality :** Calculated

$MgSiO_3$

Magnesium Silicate
Protoenstatite, syn

Lattice : Orthorhombic
S.G. : Pbcn (60)

a = 9.25000
b = 8.74000
c = 5.32000
a/b = 1.05835
c/b = 0.60870

Z = 8

Mol. weight = 100.39
Volume [CD] = 430.10
Dx = 3.101
I/Icor = 1.16

ICSD collection code: 026489
Test from ICSD: At least one TF missing.
Additional pattern: See PDF 11-273.
Sample preparation: Prepared hydrothermally.
Data collection flag: Ambient.

Smith, J.V., Acta Crystallogr., volume 12, page 515 (1959).
Calculated from ICSD using POWD-12++ (1997).

Radiation : CuKa1
Lambda : 1.54060

Filter : Not specified
d-sp : Calculated spacings

2th	i	h	k	l	2th	i	h	k	l
13.929	59	1	1	0	74.119	17	2	0	4
19.175	42	2	0	0	*74.119	17	0	6	2
20.305	80	0	2	0	74.287	10	6	2	2
21.772	487	1	1	1	74.515	4	0	2	4
26.372	371	0	2	1	74.641	9	5	5	0
27.494	177	2	1	1	74.757	20	7	1	1
28.108	999	2	2	0	74.982	68	1	6	2
*28.108	999	1	2	1	*74.982	68	2	1	4
30.724	389	3	1	0	75.397	13	1	2	4
32.187	35	1	3	0	*75.397	13	6	4	0
33.666	2	0	0	2	75.568	7	3	4	3
35.144	454	3	1	1	76.292	1	5	4	2
36.450	18	1	3	1	77.175	26	5	5	1
36.594	11	1	1	2	*77.175	26	4	5	2
39.031	244	2	0	2	77.269	25	1	5	3
39.547	15	3	2	1	77.437	58	4	6	0
39.634	10	0	2	2	*77.437	58	2	6	2
40.291	66	2	3	1	77.658	26	5	2	3
40.424	73	2	1	2	77.866	7	6	4	1
40.864	17	1	2	2	78.863	1	6	3	2
41.286	2	0	4	0	79.120	1	3	1	4
42.663	44	3	3	0	79.458	6	1	7	1
43.894	76	4	1	1	79.597	4	7	3	0
44.279	4	4	2	0	79.702	4	2	5	3
44.385	9	2	2	2	79.812	3	4	6	1
44.806	90	0	4	1	*79.812	3	1	3	4
44.972	51	3	0	2	81.249	4	7	0	2
45.922	144	2	4	0	*81.249	4	4	4	3
*45.922	144	1	4	1	81.479	3	3	6	2
46.098	81	3	3	1	81.874	4	3	2	4
46.218	37	3	1	2	*81.874	4	2	7	1
47.266	1	1	3	2	82.180	37	7	1	2
47.623	14	4	2	1	*82.180	37	5	3	3
49.154	8	2	4	1	83.550	5	8	0	0
49.811	19	3	2	2	83.846	9	6	1	3
50.378	42	5	1	0	*83.846	9	4	0	4
*50.378	42	2	3	2	84.425	31	5	5	2
52.384	42	4	0	2	84.740	25	4	1	4
53.292	45	1	5	0	85.380	1	0	4	4
53.392	68	4	3	1	85.871	12	3	7	1
*53.392	68	5	1	1	86.177	6	1	4	4
53.614	87	1	1	3	86.493	3	6	2	3
54.288	29	0	4	2	86.723	2	1	7	2
55.261	39	1	4	2	87.072	18	4	6	2
55.415	31	3	3	2	*87.072	18	8	2	0
55.911	34	0	2	3	87.418	10	4	2	4
56.234	15	1	5	1	88.288	1	7	4	1
56.522	3	2	1	3	88.563	1	2	4	4
56.755	43	4	2	2	89.109	1	2	7	2
56.865	26	1	2	3	89.549	5	8	2	1
58.027	12	4	4	0	*89.549	5	2	6	3
59.056	16	2	5	1	89.672	3	0	8	0
*59.056	16	5	3	0					
59.668	62	2	2	3					
59.954	33	6	0	0					
60.818	21	4	4	1					
*60.818	21	3	5	0					
60.952	12	5	0	2					
61.965	63	5	1	2					
*61.965	63	1	3	3					
62.685	3	3	4	2					
63.586	32	3	5	1					
63.850	57	0	6	0					
63.989	28	6	2	0					
64.531	26	1	5	2					
64.702	15	2	3	3					
64.951	21	5	2	2					
66.498	7	0	6	1					
66.633	5	6	2	1					
67.144	8	2	5	2					
67.361	13	4	1	3					
*67.361	13	1	6	1					
68.034	6	0	4	3					
68.789	2	4	4	2					
68.888	2	1	4	3					
69.649	5	4	5	1					
70.210	2	4	2	3					
70.551	16	6	0	2					
70.785	10	0	0	4					
71.401	114	6	3	1					
*71.401	114	2	4	3					
71.624	113	1	0	4					
72.251	13	7	1	0					
72.559	5	1	1	4					

Pattern : 21-1152 **Radiation =** 1.540600 **Quality :** High

$MgAl_2O_4$

Magnesium Aluminum Oxide
Spinel, syn

Lattice : Face-centered cubic
S.G. : Fd-3m (227)

a = 8.08310

Z = 8

Mol. weight = 142.27
Volume [CD] = 528.12
Dx = 3.579
I/Icor = 1.70

Color: Colorless
Sample source or locality: The sample was furnished by H.R. Shell, Bureau of Mines, College Park, Maryland, USA.
Sample preparation: Shell used a carbon electrode furnace and removed an excess of MgO with hot HCl after crushing.
Temperature of data collection: Pattern taken at 25 C.
Optical data: B=1.718
Data collection flag: Ambient.

Radiation : CuKa1
Lambda : 1.54050
SS/FOM : F29= 58(0.0151,33)

Filter : Monochromator crystal
d-sp : Not given
Internal standard : Ag

2th	i	h	k	l
19.029	35	1	1	1
31.272	40	2	2	0
36.853	100	3	1	1
38.525	4	2	2	2
44.833	65	4	0	0
55.660	10	4	2	2
59.371	45	5	1	1
65.243	55	4	4	0
68.642	4	5	3	1
74.133	4	6	2	0
77.326	8	5	3	3
78.406	2	6	2	2
82.645	6	4	4	4
85.762	2	5	5	1
90.977	6	6	4	2
94.100	12	7	3	1
99.347	8	8	0	0
107.908	2	6	6	0
111.230	8	7	5	1
112.321	2	6	6	2
116.923	6	8	4	0
120.509	2	9	1	1
121.702	2	8	4	2
126.769	2	6	6	4
130.739	8	9	3	1
138.074	18	8	4	4
142.990	2	7	7	1
152.694	2	10	2	0
160.662	12	9	5	1

Pattern : 46-1212 **Radiation =** 1.540600 **Quality :** High

Al_2O_3

Aluminum Oxide
Corundum, syn

Lattice : Rhombohedral
S.G. : R-3c (167)

Mol. weight = 101.96
Volume [CD] = 254.81
Dx = 3.987

a = 4.75870
c = 12.99290
Z = 6

Sample source or locality: The sample is an alumina plate as received from *ICDD.*
General comments: Unit cell computed from d_{obs}.
Optical data: A=1.7604, B=1.7686, Sign=-
Data collection flag: Ambient.

Huang, T., Parrish, W., Masciocchi, N., Wang, P., Adv. X-Ray Anal., volume 33, page 295 (1990).

Radiation : CuKa1
Lambda : 1.54056
SS/FOM : F25=357(0.0028,25)

Filter : Not specified
d-sp : Diffractometer

2th	i	h	k	l
25.579	45	0	1	2
35.153	100	1	0	4
37.777	21	1	1	0
41.676	2	0	0	6
43.356	66	1	1	3
46.176	1	2	0	2
52.550	34	0	2	4
57.497	89	1	1	6
59.741	1	2	1	1
61.118	2	1	2	2
61.300	14	0	1	8
66.521	23	2	1	4
68.214	27	3	0	0
70.420	1	1	2	5
74.299	2	2	0	8
76.871	29	1	0	10
77.226	12	1	1	9
80.422	1	2	1	7
80.700	2	2	2	0
83.217	1	3	0	6
84.359	3	2	2	3
85.143	1	1	3	1
86.363	2	3	1	2
86.503	3	1	2	8
88.997	9	0	2	10

Pattern : 79-1275 **Radiation =** 1.540600 **Quality :** Calculated

$Al_2(Al_{2.8}Si_{1.2})O_{9.6}$

Aluminum Silicon Oxide
Mullite, syn

Lattice : Orthorhombic
S.G. : Pbam (55)

a = 7.58800
b = 7.68800
c = 2.88950
a/b = 0.98699
c/b = 0.37585

Z = 1

Mol. weight = 316.81
Volume [CD] = 168.56
Dx = 3.121
I/Icor = 0.75

ICSD collection code: 066263
Temperature factor: ATF
Additional pattern: See PDF 15-776.
Remarks from ICSD/CSD: Model I, cell by XRD: 7.5785(6), 7.6817(7), 2.8864 (3).
Test from ICSD: Calc. density unusual but tolerable.
Data collection flag: Ambient.

Angel, R.J., McMullan, R.K., Prewitt, C.T., Am. Mineral., volume 76, page 332 (1991).
Calculated from ICSD using POWD-12++ (1997).

Radiation : CuKa1
Lambda : 1.54060

Filter : Not specified
d-sp : Calculated spacings

2th	i	h	k	l
16.401	797	1	1	0
23.120	1	0	2	0
23.429	14	2	0	0
25.963	572	1	2	0
26.171	999	2	1	0
30.922	200	0	0	1
33.150	453	2	2	0
35.197	491	1	1	1
36.995	148	1	3	0
37.399	16	3	1	0
39.157	233	2	0	1
40.805	566	1	2	1
40.945	338	2	1	1
42.536	219	2	3	0
42.761	47	3	2	0
45.964	7	2	2	1
47.254	14	0	4	0
47.915	61	4	0	0
48.842	14	1	4	0
48.963	10	1	3	1
49.286	101	3	1	1
49.447	64	4	1	0
50.669	10	3	3	0
53.394	60	2	4	0
53.508	38	2	3	1
53.697	94	3	2	1
53.849	148	4	2	0
57.546	157	0	4	1
58.123	61	4	0	1
58.936	12	1	4	1
59.469	11	4	1	1
60.550	425	3	3	1
60.691	225	4	3	0
61.482	8	1	5	0
62.312	5	5	1	0
62.988	15	2	4	1
63.399	106	4	2	1
64.440	207	0	0	2
65.443	39	2	5	0
66.146	66	5	2	0
66.998	17	1	1	2
69.444	25	0	2	2
*69.444	25	3	4	1
69.575	48	2	0	2
*69.575	48	4	4	0
70.409	125	1	5	1
70.699	56	1	2	2
70.796	68	2	1	2
71.185	36	5	1	1
71.787	21	3	5	0
72.300	15	5	3	0
73.908	17	0	6	0
74.129	125	2	5	1
74.413	80	2	2	2
74.795	130	5	2	1
75.048	89	6	0	0
76.235	20	6	1	0
76.695	37	1	3	2
76.946	28	3	1	2
78.063	17	4	4	1
78.770	4	2	6	0
79.764	9	6	2	0
80.311	32	2	3	2
*80.311	32	4	5	0
80.591	20	5	4	0
80.683	27	5	3	1
82.239	1	0	6	1
83.346	1	6	0	1
83.673	2	0	4	2
84.164	10	4	0	2
84.739	1	3	6	0
84.860	1	1	4	2
85.319	5	4	1	2
85.566	9	6	3	0
86.259	3	3	3	2
86.984	16	2	6	1
87.962	7	6	2	1
88.409	21	2	4	2
88.775	49	4	2	2
*88.775	49	5	4	1

Pattern : 85-1722 **Radiation =** 1.540600 **Quality :** Calculated

$Mg_2Al_4Si_5O_{18}$

Magnesium Aluminum Silicate
Cordierite

Lattice : Base-centered orthorhombic
S.G. : Cccm (66)

a = 17.07900
b = 9.73000
c = 9.35600
a/b = 1.75529
c/b = 0.96156
Z = 4

Mol. weight = 584.95
Volume [CD] = 1554.77
Dx = 2.499
Dm = 2.570
I/Icor = 1.02

ICSD collection code: 070110
Temperature factor: ATF
Remarks from ICSD/CSD: REM M PDF 12-303.
Remarks from ICSD/CSD: REM M Mean T-O: 1.758, 1.626, 1.614, 1.742, 1.616.
Test from ICSD: Charge sum slightly deviates from zero.
Test from ICSD: No R value given.
Temperature factor: ITF
Sample source or locality: Specimen from White Well, Australia.
Analysis: (Na0.05 K0.02 Ca0.02) (Mn0.01 Mg1.91 Fe0.08) (Si5 Al4 O18.01) (H2 O)0.56.
Additional pattern: See PDF 82-1541 and PDF 86-1550.
Data collection flag: Ambient.

Cohen, J.P., Ross, F.K., Gibbs, G.V., Am. Mineral., volume 62, page 67 (1977).
Calculated from ICSD using POWD-12++ (1997).

Radiation : CuKa1
Lambda : 1.54060
Filter : Not specified
d-sp : Calculated spacings

2th	i	h	k	l
10.351	671	2	0	0
10.455	999	1	1	0
14.108	4	1	1	1
18.038	154	3	1	0
18.221	71	0	2	0
18.955	101	0	0	2
20.398	5	3	1	1
20.787	19	4	0	0
20.999	8	2	2	0
21.695	460	2	0	2
*21.695	460	1	1	2
23.070	1	2	2	1
26.283	396	3	1	2
26.410	305	0	2	2
27.655	8	5	1	0
27.777	16	4	2	0
28.276	200	4	0	2
28.435	513	2	2	2
29.285	326	5	1	1
29.401	347	4	2	1
29.593	314	1	3	1
31.401	10	6	0	0
31.726	5	3	3	0
33.174	1	3	3	1
33.744	106	5	1	2
33.846	143	4	2	2
34.015	56	1	3	2
*34.015	56	3	1	3
35.750	1	2	2	3
36.544	34	6	2	0
36.923	38	0	4	0
*36.923	38	6	0	2
37.218	10	3	3	2
37.829	4	6	2	1
37.990	3	7	1	0
38.235	6	5	3	0
38.456	113	2	4	0
*38.456	113	0	0	4
39.235	10	7	1	1
39.474	10	5	3	1
39.681	5	2	4	1
39.961	6	2	0	4
*39.961	6	1	1	4
40.205	12	5	1	3
40.293	14	4	2	3
40.439	11	1	3	3
41.482	45	6	2	2
41.823	13	0	4	2
42.301	2	8	0	0
42.783	44	3	1	4
*42.783	44	7	1	2
42.866	34	0	2	4
43.009	36	5	3	2
43.203	47	2	4	2
*43.203	47	3	3	3
43.880	3	4	4	1
44.111	6	4	0	4
44.220	11	2	2	4
46.411	13	8	2	0
46.541	30	7	3	0
46.733	23	8	0	2
46.956	13	1	5	0
47.147	23	4	4	2
47.474	11	8	2	1
47.602	7	7	3	1
48.233	42	1	3	4
*48.233	42	7	1	3
48.436	50	5	3	3
48.612	54	2	4	3
48.858	21	9	1	0
49.234	18	6	4	0
49.458	20	3	5	0
49.882	8	1	1	5
*49.882	8	9	1	1
50.252	23	6	4	1
50.459	42	6	0	4
*50.459	42	3	5	1
50.680	52	3	3	4
*50.680	52	7	3	2
52.242	1	4	4	3
*52.242	1	3	1	5
52.865	5	9	1	2
53.220	7	6	4	2
53.432	8	3	5	2
53.619	38	10	0	0
54.092	135	6	2	4
54.203	103	5	5	0
54.372	101	0	4	4
55.166	17	5	5	1
*55.166	17	7	1	4
55.350	13	5	3	4
55.426	15	8	2	3
55.541	9	7	3	3
55.907	8	1	5	3
56.107	12	9	3	0
56.719	11	0	6	0
56.918	13	5	1	5
*56.918	13	4	2	5
57.111	22	10	2	0
57.380	13	8	4	0
*57.380	13	10	0	2
57.594	26	9	1	3
57.828	20	2	6	0
57.929	47	6	4	3
*57.929	47	5	5	2
58.130	38	3	5	3
58.298	15	8	4	1
58.486	4	8	0	4
58.840	8	4	4	4
59.207	20	0	0	6
*59.207	20	3	3	5
59.774	12	9	3	2
60.363	13	11	1	0
*60.363	13	0	6	2
60.739	11	10	2	2
61.076	5	4	6	0
61.208	3	11	1	1
61.430	1	2	6	2
61.799	23	8	2	4
61.906	34	7	3	4
*61.906	34	4	6	1
62.248	20	1	5	4
62.433	32	5	5	3
*62.433	32	3	1	6
63.308	5	7	1	5
63.543	24	5	3	5
*63.543	24	2	2	6
63.835	17	9	1	4
*63.835	17	11	1	2
64.147	4	6	4	4
*64.147	4	9	3	3
64.339	36	3	5	4
*64.339	36	7	5	2
64.569	25	4	6	2
65.352	3	8	4	3
65.534	4	12	0	0
65.767	6	2	6	3
66.279	14	6	6	0
66.627	22	5	1	6
*66.627	22	4	2	6
66.731	20	1	3	6
*66.731	20	11	3	0
67.125	3	6	6	1
67.560	1	1	7	0
*67.560	1	11	3	1
67.726	2	10	4	1
67.899	2	10	0	4
68.089	3	11	1	3
68.408	7	1	7	1
*68.408	7	5	5	4
68.653	10	12	2	0
68.904	41	12	0	2
69.079	27	9	5	0
69.485	23	8	2	5
*69.485	23	12	2	1
69.632	66	7	3	5
*69.632	66	6	6	2
70.082	11	9	3	4
*70.082	11	11	3	2
70.390	16	3	7	1
70.621	9	0	6	4
70.968	32	10	2	4
71.207	31	8	4	4
71.398	19	1	1	7
*71.398	19	9	1	5
71.619	43	2	6	4
*71.619	43	6	2	6
71.858	30	0	4	6
*71.858	30	3	5	5
72.371	7	9	5	2
72.539	15	7	1	6
*72.539	15	13	1	0
72.697	12	5	3	6
72.846	17	2	4	6
*72.846	17	3	7	2
73.497	4	5	7	0
73.724	3	6	6	3
73.843	1	11	1	4
74.164	21	11	3	3
74.301	13	10	4	3
*74.301	13	7	5	4
74.378	13	2	2	7
74.530	6	4	6	4
74.948	16	1	7	3
75.430	9	8	0	6
75.742	12	4	4	6
*75.742	12	13	1	2
75.996	7	12	2	3
76.404	8	9	5	3
*76.404	8	8	6	2
76.871	5	3	7	3
77.205	23	5	1	7
*77.205	23	4	2	7
77.361	20	1	3	7
*77.361	20	9	3	5
78.311	2	14	0	0
*78.311	2	8	2	6
78.485	3	13	3	0
*78.485	3	7	3	6

Pattern : 89-3435 **Radiation =** 1.540600 **Quality :** Calculated

SiO_2

Silicon Oxide
Cristobalite, eta

Lattice : Face-centered cubic
S.G. : Fd-3m (227)

a = 7.14700

Z = 8

Mol. weight = 60.08
Volume [CD] = 365.07
Dx = 2.186
I/Icor = 6.00

ICSD collection code: 044095
Remarks from ICSD/CSD: REM THE.
Remarks from ICSD/CSD: REM M PDF 4-359.
Test from ICSD: No R value given.
Test from ICSD: At least one TF missing.
Data collection flag: Ambient.

Feng-Liu, Garofalini, H., King-Smith, D., Vanderbilt, D., Phys. Rev. B: Condens. Matter, volume 49, page 12528 (1994).
Calculated from ICSD using POWD-12++

Radiation : CuKa1
Lambda : 1.54060

Filter : Not specified
d-sp : Calculated spacings

2th	i	h	k	l
21.518	999	1	1	1
35.498	169	2	2	0
41.889	14	3	1	1
43.846	42	2	2	2
51.077	4	4	0	0
56.043	81	3	3	1
63.742	63	4	2	2
68.117	23	5	1	1
75.135	25	4	4	0
79.231	41	5	3	1
80.583	1	4	4	2
85.947	23	6	2	0
89.943	4	5	3	3