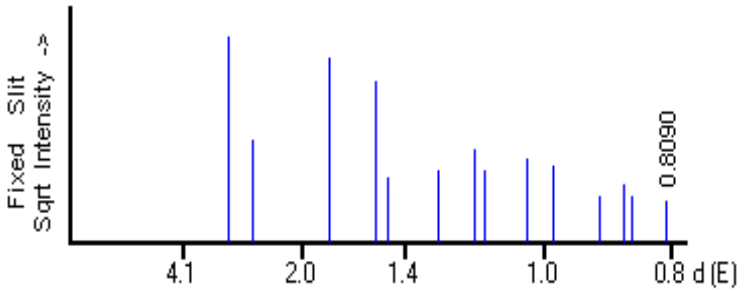
PDF # 030640, Wavelength = 0.70926 (A)

03-0640 (Deleted)
CAS Number:
Molecular Weight: 123.22
Volume[CD]: 132.89
Dx: Dm:
S.G.:
Cell Parameters:
a 5.103 b c
α β γ
SS/FOM: F14=5(0.083, 33)
I/Icor:
Rad: MoKa1
Lambda: 0.70926
Filter: ZrO2
d-sp:

Zr O2
Zirconium Oxide
Ref: Dow Chemical Co., Midland, MI, USA, Private Communication

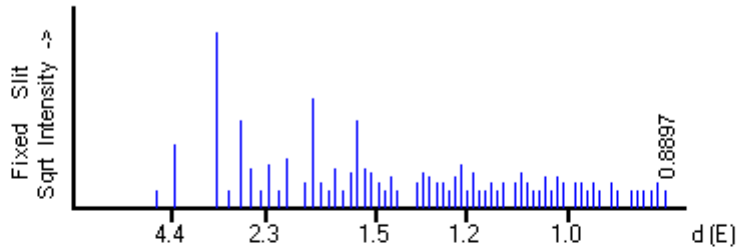


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.9600	100	1	1	1	1.2800	12	4	0	0	.90400	5	4	4	0
2.5600	24	2	0	0	1.1700	20	3	3	1	.86400	8	5	3	1
1.8100	80	2	2	0	1.1400	12	4	2	0	.85300	5	6	0	0
1.5400	60	3	1	1	1.0400	16	4	2	2	.80900	4	6	2	0
1.4800	10	2	2	2	.98400	14	5	1	1					

PDF # 411105, Wavelength = 1.540598 (A)

41-1105 Quality: *
CAS Number:
Molecular Weight: 225.81
Volume[CD]: 1192.40
Dx: 5.031 Dm:
S.G.: Ia3 (206)
Cell Parameters:
a 10.60 b c
α β γ
SS/FOM: F30=160(.0060, 31)
I/Icor: 9.1
Rad: CuKa1
Lambda: 1.540598
Filter: Graph
d-sp: diffractometer

Y2 O3
Yttrium Oxide
Ref: Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA, ICDD Grant-in-Aid, (1989)

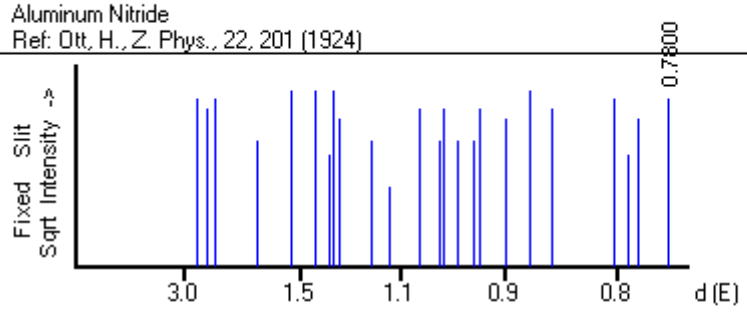


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
5.3070	<1	2	0	0	1.4705	1	6	4	0	1.0604	1	10	0	0
4.3300	13	2	1	1	1.4430	3	7	2	1	1.0500	1	10	1	1
3.0610	100	2	2	2	1.4170	1	6	4	2	1.0399	3	10	2	0
2.8350	<1	3	2	1	1.3467	2	6	5	1	1.0300	1	9	4	3
2.6510	24	4	0	0	1.3255	4	8	0	0	1.0204	3	10	2	2
2.4990	5	4	1	1	1.3052	3	8	1	1	1.0111	2	10	3	1
2.3715	1	4	2	0	1.2859	2	8	2	0	.99320	2	8	7	1
2.2605	6	3	3	2	1.2674	2	6	5	3	.98450	2	10	4	0
2.1645	1	4	2	2	1.2496	1	6	6	0	.97620	1	10	3	3
2.0788	8	4	3	1	1.2327	3	8	3	1	.96800	2	10	4	2
1.9357	2	5	2	1	1.2163	6	6	6	2	.96010	1	9	5	4
1.8740	39	4	4	0	1.2007	<1	7	5	2	.94480	2	11	2	1
1.8183	2	4	3	3	1.1856	4	8	4	0	.93740	1	8	8	0
1.7677	<1	6	0	0	1.1711	1	8	3	3	.92310	1	10	4	4
1.7200	5	6	1	1	1.1570	1	8	4	2	.91600	1	11	3	2
1.6767	1	6	2	0	1.1435	2	9	2	1	.90930	1	10	6	0
1.6361	4	5	4	1	1.1305	<1	6	6	4	.90270	1	11	4	1
1.5984	25	6	2	2	1.1178	2	8	5	1	.89630	2	10	6	2
1.5633	5	6	3	1	1.0938	2	9	3	2	.88970	<1	9	6	5
1.5304	4	4	4	4	1.0823	4	8	4	4					
1.4995	2	5	4	3	1.0712	2	9	4	1					

PDF # 031144, Wavelength = 1.5405 (A)

03-1144 (Deleted)
CAS Number:
Molecular Weight: 40.99
Volume[CD]: 41.80
Dx: 3.256 Dm: 3.050
S.G.: P63mc (186)
Cell Parameters:
a 3.113 b c 4.981
α β γ
SS/FOM: F15=2(0.240, 26)
I/Icor:
Rad: CuKa1
Lambda: 1.5405
Filter:
d-sp:

Al N
Aluminum Nitride
Ref: Ott, H., Z. Phys., 22, 201 (1924)

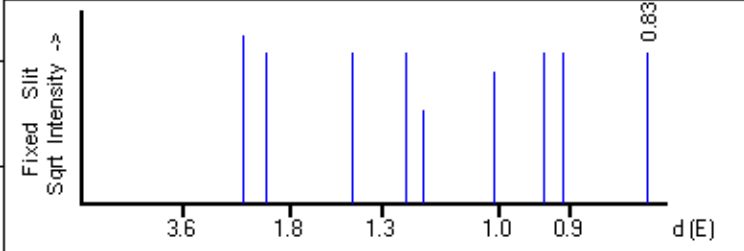


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.7000	90	1	0	0	1.3100	70				.93800	80			
2.4900	80	0	0	2	1.1900	50	2	0	2	.90100	70	3	0	0
2.3600	90	1	0	1	1.1300	20	1	0	4	.87100	100			
1.8300	50	1	0	2	1.0500	80	2	0	3	.84800	80			
1.5600	100	1	1	0	1.0100	50				.80300	90			
1.4200	100	1	0	3	1.0000	80	2	1	1	.79500	40			
1.3500	40	2	0	0	.97400	50	1	1	4	.79100	70	3	0	3
1.3300	100				.94600	50	2	1	2	.78000	90			

PDF # 030932, Wavelength = 1.5405 (A)

03-0932 (Deleted)
CAS Number:
Molecular Weight: 26.98
Volume[CD]: 65.89
Dx: 2.720 Dm:
S.G.:
Cell Parameters:
a 4.039 b c
α β γ
SS/FOM: F 6=2(0.184, 14)
I/Icor:
Rad: CuKa1
Lambda: 1.5405
Filter:
d-sp:

Al
Aluminum
Ref: Olshausen, Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem., 61, 475 (1925)

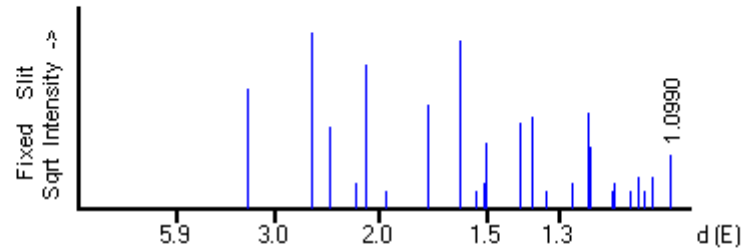


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.3200	100	1	1	1	1.2200	80	3	1	1	.93200	80			
2.0300	80	2	0	0	1.1700	30	2	2	2	.90900	80			
1.4300	80	2	2	0	1.0100	60	4	0	0	.83100	80			

PDF # 461212, Wavelength = 1.540562 (A)

46-1212 Quality: *
CAS Number:
Molecular Weight: 101.96
Volume[CD]: 254.81
Dx: 3.987 Dm:
S.G.: R$\bar{3}$c (167)
Cell Parameters:
a 4.758 b c 12.99
α β γ
SS/FOM: F25=358(.0028, 25)
I/Icor:
Rad: CuKa1
Lambda: 1.540562
Filter:
d-sp: diffractometer
Mineral Name:
Corundum, syn

α-Al2 O3
Aluminum Oxide
Ref: Huang, T et al., Adv. X-Ray Anal., 33, 295 (1990)

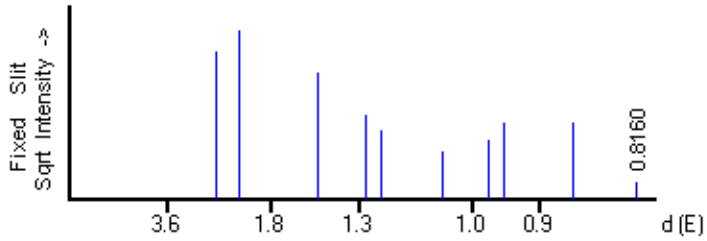


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
3.4797	45	0	1	2	1.5150	2	1	2	2	1.1897	2	2	2	0
2.5508	100	1	0	4	1.5110	14	0	1	8	1.1600	1	3	0	6
2.3794	21	1	1	0	1.4045	23	2	1	4	1.1472	3	2	2	3
2.1654	2	0	0	6	1.3737	27	3	0	0	1.1386	<1	1	3	1
2.0853	66	1	1	3	1.3359	1	1	2	5	1.1256	2	3	1	2
1.9643	1	2	0	2	1.2755	2	2	0	8	1.1241	3	1	2	8
1.7400	34	0	2	4	1.2391	29	1	0	10	1.0990	9	0	2	10
1.6015	89	1	1	6	1.2343	12	1	1	9					
1.5466	1	2	1	1	1.1931	1	2	1	7					

PDF # 060642, Wavelength = 1.5405 (A)

06-0642 (Deleted)
CAS Number:
Molecular Weight: 61.91
Volume[CD]: 76.23
Dx: 5.394 Dm: 5.250
S.G.: Fm3m (225)
Cell Parameters:
a 4.240 b c
α β γ
SS/FOM: F10=12(0.081, 10)
I/Icor:
Rad: CuKa1
Lambda: 1.5405
Filter: Ni
d-sp:
Mineral Name:
Osbornite, syn

Ti N
Titanium Nitride
Ref: Beattle, VerSnyder, Trans. Am. Soc. Met., 45, 397 (1953)

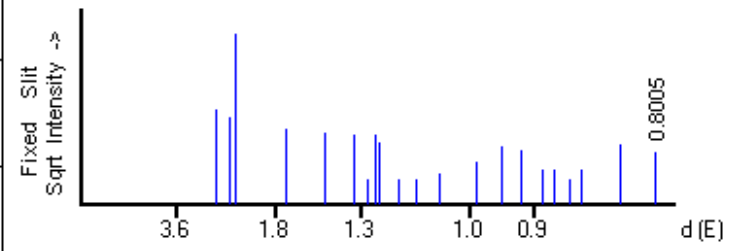


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.4400	75	1	1	1	1.2230	16	2	2	2	.86500	20	4	2	2
2.1200	100	2	0	0	1.0590	8	4	0	0	.81600	1	5	1	1
1.4960	55	2	2	0	.97200	12	3	3	1					
1.2770	25	3	1	1	.94800	20	4	2	0					

PDF # 050682, Wavelength = 1.5405 (A)

05-0682 (Deleted)
CAS Number: 7440-32-6
Molecular Weight: 47.90
Volume[CD]: 35.32
Dx: 4.504 Dm:
S.G.: P63/mmc (194)
Cell Parameters:
a 2.950 b c 4.686
α β γ
SS/FOM: F21=20(0.045, 23)
I/Icor: 1.820
Rad: CuKa1
Lambda: 1.5405
Filter: Ni
d-sp: diffractometer
Mineral Name:
Titanium, syn

Ti
Titanium
Ref: Swanson, Fuyat, Natl. Bur. Stand. (U.S.), Circ. 539, III, 4 (1954)

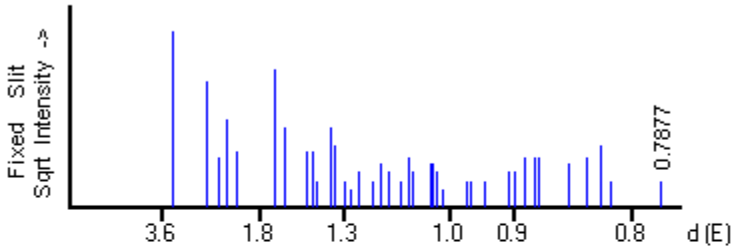


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.5570	30	1	0	0	1.2470	16	1	1	2	.91750	10	1	1	4
2.3420	26	0	0	2	1.2330	13	2	0	1	.89270	4	2	1	2
2.2440	100	1	0	1	1.1708	2	0	0	4	.87960	4	1	0	5
1.7260	19	1	0	2	1.1220	2	2	0	2	.86340	2	2	0	4
1.4750	17	1	1	0	1.0653	3	1	0	4	.85140	4	3	0	0
1.3320	16	1	0	3	.98950	6	2	0	3	.82110	12	2	1	3
1.2760	2	2	0	0	.94580	11	2	1	1	.80050	9	3	0	2

PDF # 211276, Wavelength = 1.54056 (A)

21-1276 Quality: *
CAS Number:
Molecular Weight: 79.90
Volume[CD]: 62.43
Dx: 4.250 Dm: 4.230
S.G.: P42/mnm (136)
Cell Parameters:
a 4.593 b c 2.959
α β γ
SS/FOM: F30=107(.0088, 32)
I/Icor: 3.40
Rad: CuKa1
Lambda: 1.54056
Filter:
d-sp:
Mineral Name:
Rutile, syn

Ti O2
Titanium Oxide
Ref: Natl. Bur. Stand. (U.S.) Monogr. 25, 7, 83 (1969)

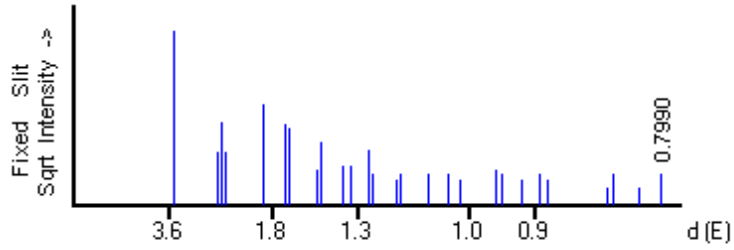


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
3.2470	100	1	1	0	1.2739	1 [	3	2	0]	.96440	2	1	0	3
2.4870	50	1	0	1	1.2441	4	2	0	2	.94380	2	1	1	3
2.2970	8	2	0	0	1.2006	2	2	1	2	.90720	4	4	0	2
2.1880	25	1	1	1	1.1702	6	3	2	1	.90090	4	5	1	0
2.0540	10	2	1	0	1.1483	4	4	0	0	.88920	8	2	1	3
1.6874	60	2	1	1	1.1143	2	4	1	0	.87740	8	4	3	1
1.6237	20	2	2	0	1.0936	8	2	2	2	.87380	8	3	3	2
1.4797	10	0	0	2	1.0827	4	3	3	0	.84370	6	4	2	2
1.4528	10	3	1	0	1.0425	6	4	1	1	.82920	8	3	0	3
1.4243	2	2	2	1	1.0364	6	3	1	2	.81960	12	5	2	1
1.3598	20	3	0	1	1.0271	4	4	2	0	.81200	2	4	4	0
1.3465	12	1	1	2	1.0167	<1 [	3	3	1]	.78770	2	5	3	0
1.3041	2	3	1	1	.97030	2	4	2	1					

PDF # 040477, Wavelength = 1.54050 (A)

04-0477 (Deleted)
CAS Number:
Molecular Weight: 79.90
Volume[CD]: 136.10
Dx: 3.899 Dm:
S.G.: I4$_1$/amd (141)
Cell Parameters:
a 3.783 b c 9.51
α β γ
SS/FOM: F25=8(0.062, 48)
I/Icor:
Rad: CuKa1
Lambda: 1.54050
Filter: Ni
d-sp: diffractometer
Mineral Name:
Anatase, syn

Ti O2
Titanium Oxide
Ref: Swanson, Tatge, Private Communication, (1950)

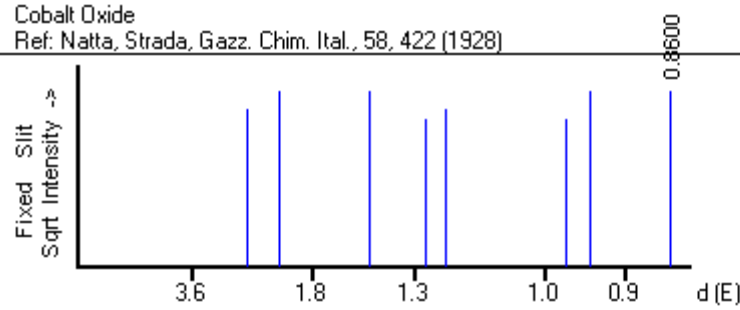


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
3.5100	100	1	0	1	1.3670	5	1	1	6	.95500	4	3	1	6
2.4350	9	1	0	3	1.3370	5	2	2	0	.94610	3	4	0	0
2.3790	22	0	0	4	1.2640	10	2	1	5	.91890	2	3	2	5
2.3360	9	1	1	2	1.2500	3	3	0	1	.89600	3	1	1	10
1.8910	33	2	0	0	1.1710	2	3	0	3	.88770	2	2	2	8
1.6990	21	1	0	5	1.1609	3	3	1	2	.83110	<1	3	2	7
1.6650	19	2	1	1	1.0869	3				.82680	3	4	1	5
1.4940	4	2	1	3	1.0433	3	3	2	1	.81000	1	3	0	9
1.4800	13	2	0	4	1.0173	2	1	0	9	.79900	3			

PDF # 021217, Wavelength = 1.54050 (A)

02-1217 (Deleted)
CAS Number:
Molecular Weight: 74.93
Volume[CD]: 75.15
Dx: 6.623 Dm: 6.455
S.G.: Fm3m (225)
Cell Parameters:
a 4.22 b c
α β γ
SS/FOM: F 4= 1 (0.314, 9)
I/Icor:
Rad:
Lambda:
Filter:
d-sp:

Co O
Cobalt Oxide
Ref: Natta, Strada, Gazz. Chim. Ital., 58, 422 (1928)

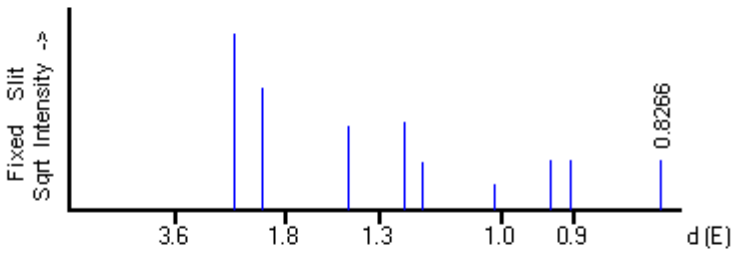


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.4700	80				1.2700	70	3	1	1	.94000	100			
2.0900	100	2	0	0	1.2100	80				.86000	100	4	2	2
1.4800	100				.97000	70	3	3	1					

PDF # 040787, Wavelength = 1.54056 (A)

04-0787 Quality: *
CAS Number: 7429-90-5
Molecular Weight: 26.98
Volume[CD]: 66.40
Dx: 2.699 Dm:
S.G.: Fm3m (225)
Cell Parameters:
a 4.049 b c
α β γ
SS/FOM: F 9=93(.0108, 9)
I/Icor: 3.619
Rad: CuKa1
Lambda: 1.54056
Filter: Ni
d-sp:
Mineral Name:
Aluminum, syn [NR]

Al
Aluminum
Ref: Swanson, Tatge, Natl. Bur. Stand. (U.S.), Circ. 539, I, 11 (1953)

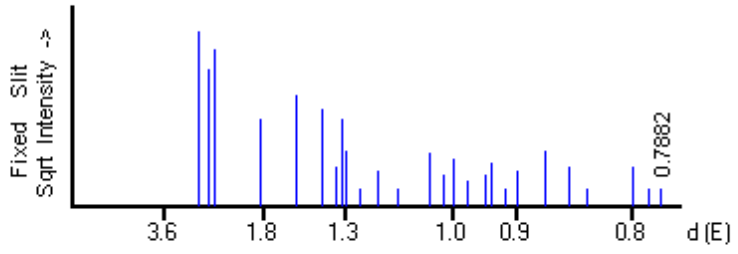


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.3380	100	1	1	1	1.2210	24	3	1	1	.92890	8	3	3	1
2.0240	47	2	0	0	1.1690	7	2	2	2	.90550	8	4	2	0
1.4310	22	2	2	0	1.0124	2	4	0	0	.82660	8	4	2	2

PDF # 251133, Wavelength = 1.540598 (A)

25-1133 Quality: *
CAS Number: 24304-00-5
Molecular Weight: 40.99
Volume[CD]: 41.74
Dx: 3.261 Dm:
S.G.: P63mc (186)
Cell Parameters:
a 3.111 b c 4.979
α β γ
SS/FOM: F26=80(.0117, 28)
I/Icor: 1.60
Rad: CuKa1
Lambda: 1.540598
Filter:
d-sp:

Al N
Aluminum Nitride
Ref: Natl. Bur. Stand. (U.S.) Monogr. 25, 12, 5 (1975)

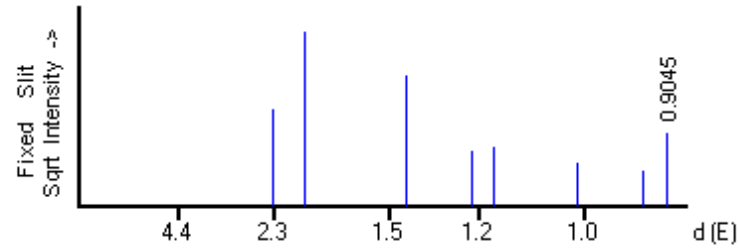


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.6950	100	1	0	0	1.2450	1	0	0	4	.91420	<1	2	0	4
2.4900	60	0	0	2	1.1850	4	2	0	2	.89820	4	3	0	0
2.3710	80	1	0	1	1.1301	1	1	0	4	.86800	10	2	1	3
1.8290	25	1	0	2	1.0461	9	2	0	3	.84480	5	3	0	2
1.5559	40	1	1	0	1.0184	3	2	1	0	.82980	1	0	0	6
1.4133	30	1	0	3	.99780	7	2	1	1	.80080	5	2	0	5
1.3475	5	2	0	0	.97200	2	1	1	4	.79310	1	1	0	6
1.3194	25	1	1	2	.94250	3	2	1	2	.78820	<1	2	1	4
1.3007	10	2	0	1	.93400	6	1	0	5					

PDF # 461200, Wavelength = 1.5418 (A)

46-1200 Quality: *
CAS Number:
Molecular Weight: 40.99
Volume[CD]: 66.18
Dx: 4.113 Dm:
S.G.: Fm3m (225)
Cell Parameters:
a 4.045 b c
α β γ
SS/FOM: F 8=155(.0064, 8)
I/Icor:
Rad: CuKa
Lambda: 1.5418
Filter:
d-sp: diffractometer

Al N
Aluminum Nitride
Ref: Vollstadt, H et al., Proc. Jpn. Acad., Ser. B, 66, 7 (1990)

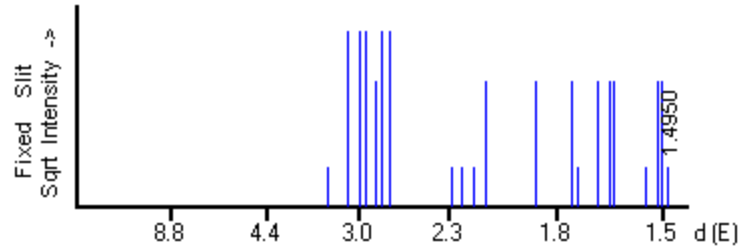


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.3346	30	1	1	1	1.2195	10	3	1	1	.92800	4	3	3	1
2.0226	100	2	0	0	1.1678	11	2	2	2	.90450	17	4	2	0
1.4300	55	2	2	0	1.0113	6	4	0	0					

PDF # 471274, Wavelength = 1.5418 (A)

47-1274 Quality: I
CAS Number:
Molecular Weight: 225.81
Volume[CD]: 414.25
Dx: 5.431 Dm:
S.G.: C2/m (12)
Cell Parameters:
a 13.88 b 3.513 c 8.629
α β 100.09 γ
SS/FOM: F21=4(0.057, 88)
I/Icor:
Rad: CuKa
Lambda: 1.5418
Filter:
d-sp: diffractometer

β-Y2 O3
Yttrium Oxide
Ref: Atou, T et al., J. Solid State Chem., 89, 378 (1990)

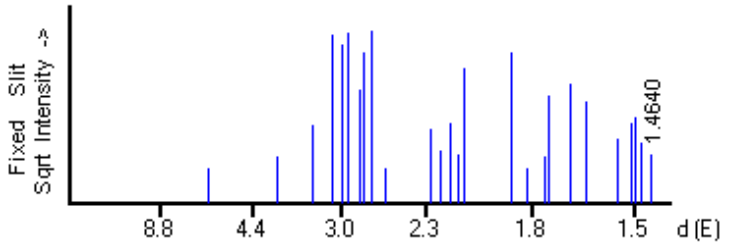


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
3.3700	5 [	4	0	$\bar{1}$]	2.2790	5	6	0	0	1.6740	50	7	1	$\bar{2}$
3.1200	100	1	1	1	2.2280	5	1	1	$\bar{3}$	1.6380	50	4	0	$\bar{5}$
3.0000	100	4	0	1	2.1630	5	5	1	$\bar{1}$	1.6280	50	7	1	1
2.9360	100	4	0	$\bar{2}$	2.1030	50	3	1	$\bar{3}$	1.5470	5	1	1	$\bar{5}$
2.8360	50	0	0	3	1.8870	50	3	1	3	1.5140	50	4	2	1
2.7890	100	3	1	0	1.7540	50	0	2	0	1.5060	50	4	2	$\bar{2}$
2.7210	100	1	1	$\bar{2}$	1.7340	5	8	0	$\bar{1}$	1.4950	5	8	0	2

PDF # 440399, Wavelength = 1.5418 (A)

44-0399 Quality: I
CAS Number:
Molecular Weight: 225.81
Volume[CD]: 411.45
Dx: 5.468 Dm: 4.980
S.G.: C2/m (12)
Cell Parameters:
a 13.89 b 3.493 c 8.611
α β 100.27 γ
SS/FOM: F26=21(.0139, 91)
I/Icor:
Rad: CuKa
Lambda: 1.5418
Filter: Graph
d-sp: diffractometer

Y2 O3
Yttrium Oxide
Ref: Vogt, G., Proc.-Electrochem. Soc., 572 (1988)

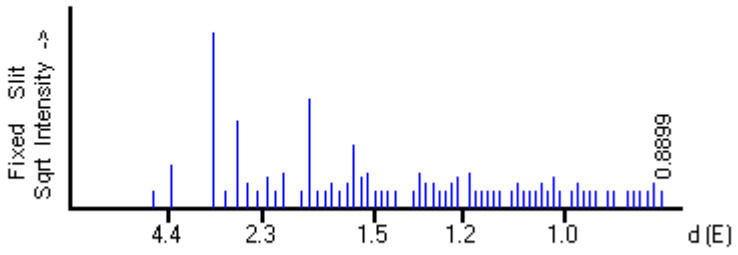


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
5.8580	4	2	0	$\bar{1}$	2.5890	4	1	1	2	1.7470	38	0	2	0
3.9300	7	2	0	$\bar{2}$	2.2800	18	6	0	0	1.6740	47	7	1	$\bar{2}$
3.3460	20	2	0	2	2.2170	9	1	1	$\bar{3}$	1.6250	34	7	1	1
3.0970	95	1	1	1	2.1620	21	5	1	$\bar{1}$	1.5430	14	1	1	$\bar{5}$
2.9920	83	4	0	1	2.1200	8	0	0	4	1.5080	21	4	2	1
2.9290	96	4	0	$\bar{2}$	2.0950	61	3	1	$\bar{3}$	1.5000	25	4	2	$\bar{2}$
2.8240	43	0	0	3	1.8790	75	3	1	3	1.4860	12	0	2	3
2.7740	75	3	1	0	1.8190	4	5	1	2	1.4640	8	8	0	4
2.7040	100	1	1	$\bar{2}$	1.7600	7	1	1	4					

PDF # 431036, Wavelength = 1.54056 (A)

43-1036 Quality: C
CAS Number:
Molecular Weight: 225.81
Volume[CD]: 1192.36
Dx: 5.032 Dm:
S.G.: Ia3 (206)
Cell Parameters:
a 10.60 b c
α β γ
SS/FOM: F30=561(.0017, 31)
I/Icor: 8.60
Rad: CuKa1
Lambda: 1.54056
Filter:
d-sp: calculated

Y2 O3
Yttrium Oxide
Ref: Grier, D., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA, ICDD Grant-in-Aid, (1991)

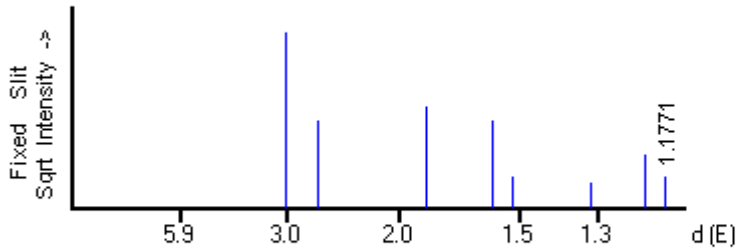


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
5.3020	<1	2	0	0	1.4996	1	5	4	3	1.0712	1	8	5	3
4.3290	6	2	1	1	1.4705	1	0	4	6	1.0604	1	8	6	0
3.0610	100	2	2	2	1.4430	1	7	2	1	1.0500	<1	10	1	1
2.8340	<1	1	2	3	1.4170	1	6	4	2	1.0398	2	2	6	8
2.6510	25	4	0	0	1.3467	1	6	5	1	1.0300	<1	3	4	9
2.4990	2	4	1	1	1.3255	4	8	0	0	1.0204	3	10	2	2
2.3710	1	4	2	0	1.3053	2	7	4	1	1.0111	1	7	6	5
2.2610	3	3	3	2	1.2859	2	8	2	0	.99320	1	8	5	5
2.1650	<1	4	2	2	1.2674	1	6	5	3	.98460	2	0	4	10
2.0800	4	1	3	4	1.2497	1	8	2	2	.97620	1	1	6	9
1.9360	1	5	2	1	1.2327	2	8	3	1	.96800	1	10	4	2
1.8745	39	4	4	0	1.2164	3	6	6	2	.96000	1	8	7	3
1.8186	1	4	3	3	1.1856	4	8	4	0	.94470	1	10	5	1
1.7673	<1	6	0	0	1.1710	<1	8	3	3	.93730	1	8	8	0
1.7202	2	6	1	1	1.1570	1	2	4	8	.92300	1	10	4	4
1.6766	1	0	2	6	1.1435	1	6	5	5	.91600	1	10	5	3
1.6362	2	1	4	5	1.1304	<1	6	6	4	.90930	1	8	6	6
1.5986	13	6	2	2	1.1178	1	1	5	8	.90270	1	8	7	5
1.5635	3	1	3	6	1.0937	1	7	6	3	.89620	2	10	6	2
1.5306	4	4	4	4	1.0823	2	8	4	4	.88990	<1	9	6	5

PDF # 430661, Wavelength = 1.54060 (A)

43-0661 Quality: *
CAS Number:
Molecular Weight: 225.81
Volume[CD]: 145.90
Dx: 5.140 Dm:
S.G.: Fm3 (202)
Cell Parameters:
a 5.264 b c
α β γ
SS/FOM: F 8=79(.0127, 8)
I/Icor:
Rad: CuKa1
Lambda: 1.54060
Filter: Graph
d-sp: diffractometer

Y2 O3
Yttrium Oxide
Ref: Katagiri, S., Ishizawa, N., Marumo, F., Powder Diffraction, 8, 60 (1993)

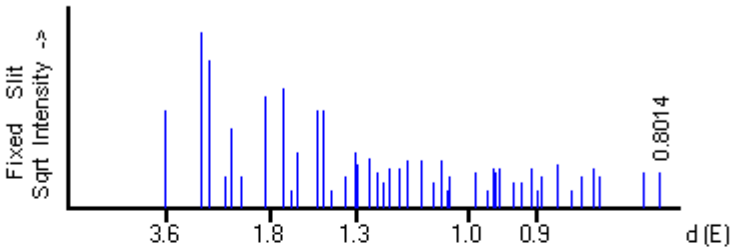


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
3.0346	100	1	1	1	1.5870	24	3	1	1	1.2079	9	3	3	1
2.6318	24	2	0	0	1.5200	3	2	2	2	1.1771	3	2	4	0
1.8615	33	2	2	0	1.3161	2	4	0	0					

PDF # 330664, Wavelength = 1.540598 (A)

33-0664 Quality: *
CAS Number: 1309-37-1
Molecular Weight: 159.69
Volume[CD]: 301.93
Dx: 5.270 Dm: 5.260
S.G.: R$\bar{3}$c (167)
Cell Parameters:
a 5.035 b c 13.74
α β γ
SS/FOM: F30=69(.0111, 39)
I/Icor: 2.4
Rad: CuKa1
Lambda: 1.540598
Filter:
d-sp: diffractometer
Mineral Name:
Hematite, syn

Fe2 O3
Iron Oxide
Ref: Natl. Bur. Stand. (U.S.) Monogr. 25, 18, 37 (1981)

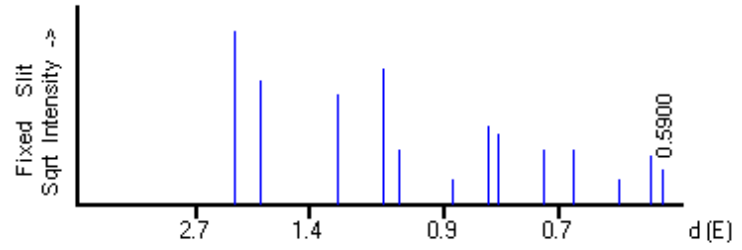


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
3.6840	30	0	1	2	1.3115	10	1	0	10	.96060	5	3	2	4
2.7000	100	1	0	4	1.3064	6	1	1	9	.95810	4	0	1	14
2.5190	70	1	1	0	1.2592	8	2	2	0	.95160	5	4	1	0
2.2920	3	0	0	6	1.2276	4	3	0	6	.93180	2	4	1	3
2.2070	20	1	1	3	1.2141	2	2	2	3	.92060	2	0	4	8
2.0779	3	2	0	2	1.1896	5	1	2	8	.90810	5	1	3	10
1.8406	40	0	2	4	1.1632	5	0	2	10	.89980	1	3	0	12
1.6941	45	1	1	6	1.1411	7	1	3	4	.89540	3	2	0	14
1.6367	1	2	1	1	1.1035	7	2	2	6	.87890	6	4	1	6
1.6033	5	1	2	2	1.0768	2	0	4	2	.86480	1	2	3	8
1.5992	10	0	1	8	1.0557	7	2	1	10	.85430	3	4	0	10
1.4859	30	2	1	4	1.0428	<1	1	1	12	.84360	5	1	2	14
1.4538	30	3	0	0	1.0393	3	4	0	4	.83920	3	3	3	0
1.4138	<1	[1	2	5]	.98920	4	3	1	8	.80890	4	3	2	10
1.3497	3	2	0	8	.97150	<1	2	2	9	.80140	4	2	4	4

PDF # 011258, Wavelength = 0.709 (A)

01-1258 (Deleted)
CAS Number:
Molecular Weight: 58.70
Volume[CD]: 44.36
Dx: 4.394 Dm: 8.720
S.G.: Fm3m (225)
Cell Parameters:
a 3.540 b c
α β γ
SS/FOM: F12=8(0.116, 13)
I/Icor:
Rad: MoKa
Lambda: 0.709
Filter:
d-sp:

Ni
Nickel
Ref: Hull, Phys. Rev., 17, 571 (1921)

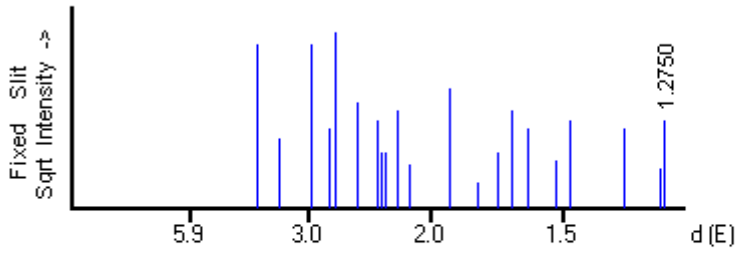


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.0400	100	1	1	1	.88000	2	4	0	0	.63000	2			
1.7700	50	2	0	0	.81000	20	3	3	1	.60000	8	5	3	1
1.2500	40	2	2	0	.79000	16	4	2	0	.59000	4	6	0	0
1.0700	60	3	1	1	.72000	10	4	2	2					
1.0200	10	2	2	2	.68000	10	5	1	1					

PDF # 310806, Wavelength = 1.54056 (A)

31-0806 Quality: *
CAS Number:
Molecular Weight: 151.26
Volume[CD]: 227.37
Dx: 4.419 Dm:
S.G.: Pnma (62)
Cell Parameters:
a 5.924 b 7.666 c 5.005
α β γ
SS/FOM: F22=28(.0119, 65)
I/Icor:
Rad: CuKa1
Lambda: 1.54056
Filter: Ni
d-sp:

Mg Se O3
Magnesium Selenate
Ref: Kohn, K., Waseda University, Tokyo, Japan, Private Communication

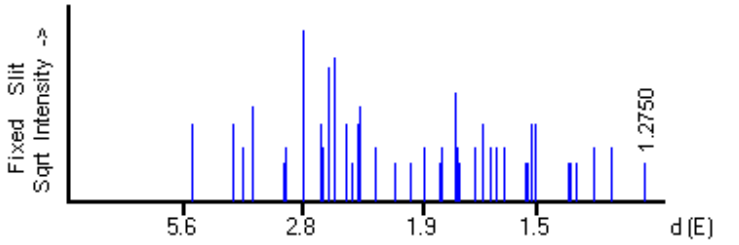


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
3.8300	85	0	2	0	2.2770	10	0	3	1	1.6090	20	2	4	0
3.4200	15	1	1	1	2.2080	30	1	1	2	1.5220	7	0	4	2
2.9630	85	2	0	0	2.1240	6	1	3	1	1.4810	25	4	0	0
2.7640	20	2	1	0	1.9160	35	0	4	0	1.3540	20	2	4	2
2.7080	100	1	2	1	1.9120	45	2	0	2	1.2810	5	4	3	0
2.5030	35	0	0	2	1.7860	2	3	1	1	1.2750	25	4	0	2
2.3440	25	2	2	0	1.7120	10	1	3	2					
2.3050	10	1	0	2	1.6570	30	3	2	1					

PDF # 310633, Wavelength = 1.9373 (A)

31-0633 Quality: I
CAS Number:
Molecular Weight: 203.78
Volume[CD]: 302.40
Dx: 3.908 Dm: 3.880
S.G.: Pbnm (62)
Cell Parameters:
a 4.799 b 10.39 c 6.063
α β γ
SS/FOM: F30=24(0.028, 45)
I/Icor:
Rad: FeKa
Lambda: 1.9373
Filter: Mn
d-sp:
Mineral Name:
Fayalite, magnesian

(Fe , Mg)2 Si O4
Iron Magnesium Silicate
Ref: Gillery, College of Min. Ind., Penn State Univ., University Park, PA, USA, Private Communication

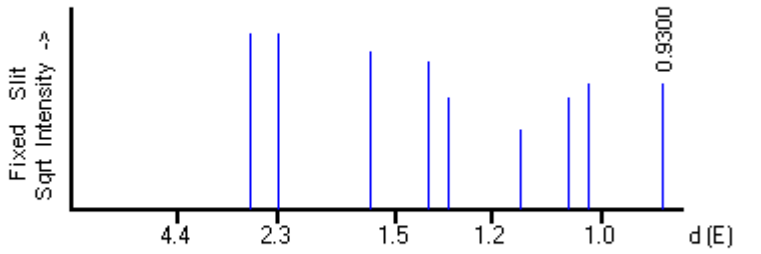


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
5.2100	20	0	2	0	2.2970	20	1	2	2	1.6150	10	1	5	2
3.9450	20	0	2	1	2.2860	30	1	4	0	1.5950	10	0	4	3
3.7620	10	1	0	1	2.1840	10	2	1	1	1.5310	5	3	1	1
3.5350	30	1	1	1	2.0620	5	1	3	2	1.5250	5	2	4	2
3.0450	5	1	2	1	1.9740	5	0	4	2	1.5150	20	0	0	4
3.0270	10	0	0	2	1.9080	10	1	5	0	1.5040	20	0	6	2
2.8100	100	1	3	0	1.8340	5	1	1	3	1.4190	5	1	7	0
2.6160	20	0	2	2	1.8200	10	1	5	1	1.4140	5	3	3	1
2.5990	10	0	4	0	1.7690	40	2	2	2	1.4030	5	3	1	2
2.5490	60	1	3	1	1.7610	10	2	4	0	1.3670	10	2	6	1
2.4890	70	1	1	2	1.7530	5	1	2	3	1.3330	10	1	3	4
2.4000	5	2	0	0	1.6930	10	2	4	1	1.2750	5	2	6	2
2.3890	20	0	4	1	1.6650	20	0	6	1					
2.3400	5	2	1	0	1.6400	10	1	3	3					

PDF # 020956, Wavelength = 1.542 (A)

02-0956 Quality:
CAS Number:
Molecular Weight: 105.23
Volume[CD]: 94.82
Dx: 7.371 Dm:
S.G.: Fm3m (225)
Cell Parameters:
a 4.56 b c
α β γ
SS/FOM: F 9=5(0.194, 9)
I/Icor:
Rad: CuKa
Lambda: 1.542
Filter:
d-sp:

Zr N
Zirconium Nitride
Ref: General Electric Company, Wembley, England, UK, Private Communication

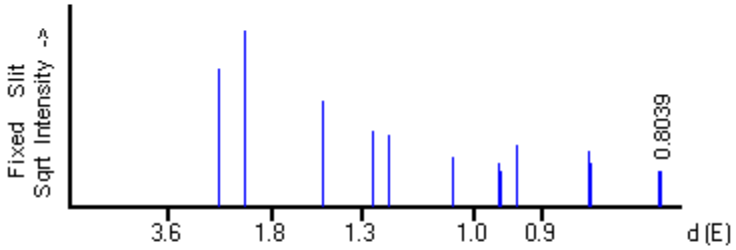


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.6400	100	1	1	1	1.3800	70	3	1	1	1.0500	40	3	3	1
2.2900	100	2	0	0	1.3200	40	2	2	2	1.0200	50	4	2	0
1.6200	80	2	2	0	1.1400	20	4	0	0	.93000	50	4	2	2

PDF # 221189, Wavelength = 1.54056 (A)

22-1189 (Deleted)
CAS Number: 1313-99-1
Molecular Weight: 74.70
Volume[CD]: 54.68
Dx: 6.805 Dm:
S.G.: R$\bar{3}$m (166)
Cell Parameters:
a 2.954 b c 7.236
α β γ
SS/FOM: F17=13(0.056, 23)
I/Icor:
Rad: CuKa1
Lambda: 1.54056
Filter: Ni
d-sp:

Ni O
Nickel Oxide
Ref: Toussaint, C., Euratom, Ispra, Italia, Private Communication, (1969)

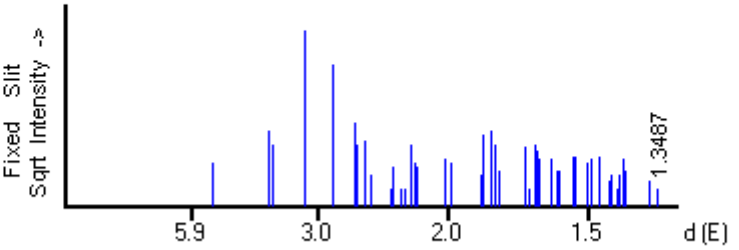


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.4120	60	0	0	3	1.2064	16	0	0	6	.93370	10	1	2	2
2.0880	100	0	1	2	1.0445	8	0	2	4	.85290	10	0	1	8
1.4770	35	1	0	4	.95880	6	1	0	7	.85190	6	3	0	0
1.4760	35	1	1	0	.95810	4	2	0	5	.80410	4	0	0	9
1.2600	18	0	1	5	.95760	4	2	1	1	.80390	4	3	0	3
1.2586	12	0	2	1	.93450	12	1	1	6					

PDF # 360420, Wavelength = 1.54178 (A)

36-0420 (Deleted)
CAS Number:
Molecular Weight: 123.22
Volume[CD]: 140.66
Dx: 5.818 Dm: 5.710
S.G.: P2$_1$/c (14)
Cell Parameters:
a 5.146 b 5.213 c 5.311
α β 99.2 γ
SS/FOM: F30=63(.0140, 34)
I/Icor: 2.6
Rad: CuKa
Lambda: 1.54178
Filter: Graph
d-sp: diffractometer
Mineral Name:
Baddeleyite, syn

Zr O2
Zirconium Oxide
Ref: Larson, F., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA, ICDD Grant-in-Aid, (1985)



d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
5.0790	6	1	0	0	1.9910	6	$\bar{2}$	0	2	1.5455	8	1	3	1
3.6940	18	0	1	1	1.8593	3	$\bar{2}$	1	2	1.5392	8	$\bar{3}$	0	2
3.6360	12	$\bar{1}$	1	0	1.8480	16	0	2	2	1.5088	6	1	1	3
3.1630	100	$\bar{1}$	1	1	1.8186	18	$\bar{2}$	2	0	1.4956	7	$\bar{2}$	1	3
2.8390	64	1	1	1	1.8032	12	$\bar{1}$	2	2	1.4769	8	3	1	1
2.6200	22	0	0	2	1.7825	4	$\bar{2}$	2	1	1.4769	8	$\bar{3}$	1	2
2.6050	12	0	2	0	1.6934	11	2	0	2	1.4514	2	0	2	3
2.5400	14	$\bar{2}$	0	0	1.6934	11	3	0	0	1.4474	3	0	3	2
2.4970	3	$\bar{1}$	0	2	1.6768	<1	1	2	2	1.4474	3	$\bar{1}$	2	3
2.3420	1	0	1	2	1.6603	8	2	2	1	1.4336	<1	$\bar{2}$	3	0
2.3320	5	0	2	1	1.6567	12	0	1	3	1.4260	3	$\bar{1}$	3	2
2.2830	1	$\bar{2}$	1	0	1.6508	10	$\bar{1}$	1	3	1.4197	7	2	2	2
2.2530	1	[$\bar{1}$	1	2]	1.6483	5	0	3	1	1.4197	7	$\bar{3}$	2	0
2.2131	12	$\bar{2}$	1	1	1.6434	7	$\bar{1}$	3	0	1.4158	4	$\bar{2}$	3	1
2.1905	6	1	0	2	1.6104	7	2	1	2	1.3610	2	1	3	2
2.1800	5	$\bar{1}$	2	1	1.6104	7	$\bar{3}$	1	0	1.3487	<1	1	2	3
2.0191	7	1	1	2	1.5916	4	$\bar{1}$	3	1					
1.9910	6	2	1	1	1.5819	4	$\bar{2}$	2	2					

PDF # 310633, Wavelength = 1.9373 (A)

31-0633 Quality: I

CAS Number:

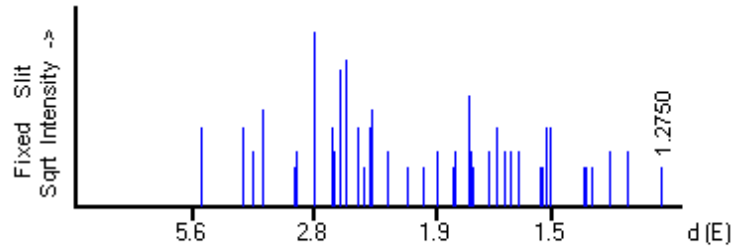
Molecular Weight: 203.78
Volume[CD]: 302.40
Dx: 3.908 Dm: 3.880

S.G.: Pbnm (62)
Cell Parameters:
a 4.799 b 10.39 c 6.063
α β γ

SS/FOM: F30=24(0.028, 45)
I/Icor:
Rad: FeKa
Lambda: 1.9373
Filter: Mn
d-sp:

Mineral Name:
Fayalite, magnesian

(Fe , Mg)2 Si O4
Iron Magnesium Silicate
Ref: Gillery, College of Min. Ind., Penn State Univ., University Park, PA, USA, Private Communication



d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
5.2100	20	0	2	0	2.2970	20	1	2	2	1.6150	10	1	5	2
3.9450	20	0	2	1	2.2860	30	1	4	0	1.5950	10	0	4	3
3.7620	10	1	0	1	2.1840	10	2	1	1	1.5310	5	3	1	1
3.5350	30	1	1	1	2.0620	5	1	3	2	1.5250	5	2	4	2
3.0450	5	1	2	1	1.9740	5	0	4	2	1.5150	20	0	0	4
3.0270	10	0	0	2	1.9080	10	1	5	0	1.5040	20	0	6	2
2.8100	100	1	3	0	1.8340	5	1	1	3	1.4190	5	1	7	0
2.6160	20	0	2	2	1.8200	10	1	5	1	1.4140	5	3	3	1
2.5990	10	0	4	0	1.7690	40	2	2	2	1.4030	5	3	1	2
2.5490	60	1	3	1	1.7610	10	2	4	0	1.3670	10	2	6	1
2.4890	70	1	1	2	1.7530	5	1	2	3	1.3330	10	1	3	4
2.4000	5	2	0	0	1.6930	10	2	4	1	1.2750	5	2	6	2
2.3890	20	0	4	1	1.6650	20	0	6	1					
2.3400	5	2	1	0	1.6400	10	1	3	3					

PDF # 310795, Wavelength = 1.9373 (A)

31-0795 Quality: I

CAS Number:

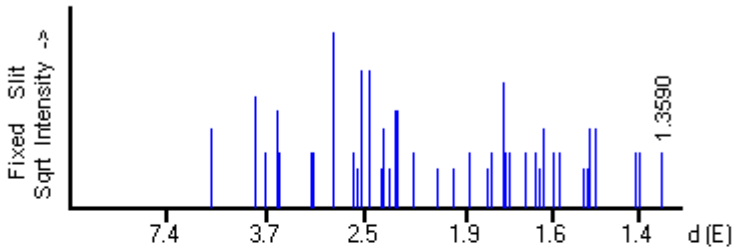
Molecular Weight: 140.69
Volume[CD]: 297.50
Dx: 3.648 Dm: 3.690

S.G.: Pbnm (62)
Cell Parameters:
a 4.784 b 10.31 c 6.027
α β γ

SS/FOM: F30=25(0.029, 42)
I/Icor:
Rad: FeKa
Lambda: 1.9373
Filter: Mn
d-sp:

Mineral Name:
Forsterite, ferroan

(Mg , Fe)2 Si O4
Magnesium Iron Silicate
Ref: Gillery, College of Min. Ind., Penn State Univ., University Park, PA, USA, Private Communication



d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
5.1500	20	0	2	0	2.3300	5	2	1	0	1.6440	5	2	3	2
3.9160	40	0	2	1	2.2850	30	1	2	2	1.6310	20	1	3	3
3.7440	10	1	0	1	2.2700	30	1	4	0	1.6040	10	1	5	2
3.5160	30	1	1	1	2.1730	10	2	1	1	1.5860	10	0	4	3
3.4810	10	1	2	0	2.0480	5	1	3	2	1.5230	5	3	2	0
3.0300	10	1	2	1	1.9620	5	2	3	0	1.5130	5	2	5	1
3.0140	10	0	0	2	1.8940	10	1	5	0	1.5080	20	0	0	4
2.7910	100	1	3	0	1.8230	5	1	1	3	1.4940	20	0	6	2
2.6010	10	0	2	2	1.8070	10	1	5	1	1.4080	10u	1	7	0
2.5780	5	0	4	0	1.7610	50	2	2	2	1.4060	u	2	3	3
2.5330	60	1	3	1	1.7540	10	2	4	0	1.3970	10	3	1	2
2.4750	60	1	1	2	1.7430	10	1	2	3	1.3590	10	3	2	2
2.3910	5	2	0	0	1.6840	10	2	4	1					
2.3700	20	0	4	1	1.6540	10	0	6	1					

PDF # 190771, Wavelength = 1.5405 (A)

19-0771 Quality: O

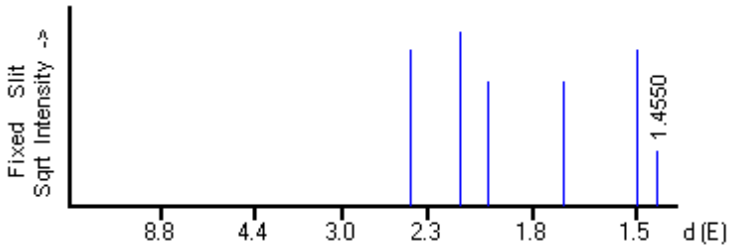
CAS Number:

Molecular Weight: 56.30
Volume[CD]:
Dx: Dm:

S.G.:
Cell Parameters:
a b c
α β γ

SS/FOM: F = (,)
I/Icor:
Rad: CuKa1
Lambda: 1.5405
Filter:
d-sp:

Mg O2
Magnesium Oxide
Ref: Allamagny, Rev. Chim. Miner., 2, 645 (1965)



d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.4200	80				1.9850	50				1.4990	80			
2.1200	100				1.7000	50				1.4550	10			

PDF # 461237, Wavelength = 1.5406 (A)

46-1237 Quality: R

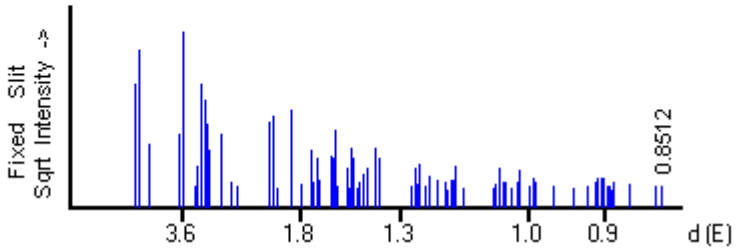
CAS Number:

Molecular Weight: 79.90
Volume[CD]: 285.45
Dx: 3.718 Dm:

S.G.: C2/m (12)
Cell Parameters:
a 12.20 b 3.748 c 6.535
α β 107.36 γ

SS/FOM: F30=66(.0082, 55)
I/Icor:
Rad: CuKa1
Lambda: 1.54063
Filter: Ge
d-sp: calculated

β-Ti O2
Titanium Oxide
Ref: Kaduk, J., Chen, Y.-M., Amoco Corporation, Naperville, IL, USA, Private Communication, (1994)

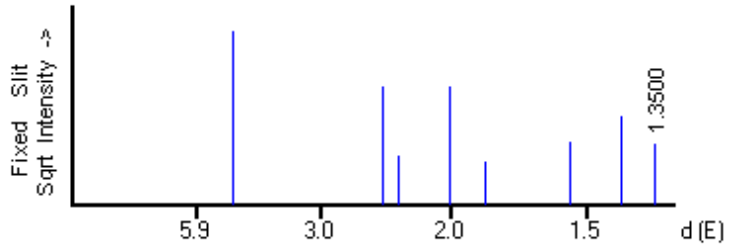


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
6.2350	490	0	0	1	1.5208	47	7	1	$\bar{0}$	1.0570	18	6	0	$\bar{6}$
5.8236	793	2	0	$\bar{0}$	1.5082	11	4	2	$\bar{2}$	1.0517	47	3	1	5
5.0806	124	2	0	$\bar{1}$	1.5022	111	3	1	3	1.0517	47	1	3	$\bar{3}$
3.7351	172	2	0	1	1.4936	21	4	0	$\bar{3}$	1.0452	20	3	1	$\bar{6}$
3.5685	999	1	1	$\bar{0}$	1.4902	80	3	1	$\bar{4}$	1.0429	16	9	1	2
3.2272	13	1	1	$\bar{1}$	1.4724	11	4	2	1	1.0382	21	0	2	$\bar{5}$
3.1711	52	2	0	$\bar{2}$	1.4632	20	6	0	$\bar{2}$	1.0309	11	9	1	$\bar{5}$
3.1175	495	0	0	$\bar{2}$	1.4444	36	6	0	$\bar{4}$	1.0206	20	10	2	$\bar{2}$
3.0051	367	4	0	$\bar{1}$	1.4272	49	7	1	$\bar{3}$	1.0161	21	10	0	$\bar{5}$
2.9816	218	1	1	1	1.3919	110	0	2	$\bar{3}$	1.0155	42	7	3	$\bar{1}$
2.9118	105	4	0	0	1.3784	75	6	2	$\bar{1}$	.99920	13	7	3	0
2.6968	147	3	1	$\bar{0}$	1.2647	15	6	2	1	.99388	29	3	3	$\bar{3}$
2.6868	169	3	1	$\bar{1}$	1.2566	47	6	2	$\bar{3}$	.99039	21	3	3	$\bar{4}$
2.5403	20	4	0	$\bar{2}$	1.2470	16	0	0	5	.98930	13	10	2	0
2.4595	15	2	0	2	1.2424	38	3	1	4	.96472	13	7	1	4
2.0783	236	0	0	3	1.2424	38	1	3	0	.93721	12	0	4	$\bar{0}$
2.0341	263	6	0	$\bar{1}$	1.2398	61	7	1	2	.92073	15	6	2	$\bar{6}$
1.9974	11	4	0	$\bar{3}$	1.2233	14	9	1	$\bar{0}$	.91070	21	13	1	$\bar{2}$
1.8742	302	0	2	0	1.2105	33	4	2	$\bar{4}$	.90844	27	3	1	6
1.7949	17	2	0	3	1.1890	22	3	3	$\bar{0}$	.90545	26	7	3	$\bar{2}$
1.7949	17	0	2	1	1.1890	22	3	3	$\bar{1}$	.90350	26	3	1	$\bar{7}$
1.7284	103	1	1	3	1.1681	20	4	2	3	.89963	15	13	1	$\bar{1}$
1.7137	21	6	0	$\bar{1}$	1.1647	10	10	0	0	.89753	15	0	4	$\bar{2}$
1.6935	75	6	0	$\bar{3}$	1.1534	24	6	2	2	.89471	10	4	4	$\bar{1}$
1.6753	23	2	2	1	1.1492	24	3	3	$\bar{1}$	.89331	21	10	2	$\bar{5}$
1.6064	86	0	2	$\bar{2}$	1.1469	16	3	3	$\bar{2}$	.87695	16	13	1	$\bar{4}$
1.5904	78	4	2	$\bar{1}$	1.1444	55	1	1	$\bar{5}$	.85436	15	0	4	$\bar{3}$
1.5855	123	4	0	$\bar{4}$	1.1444	55	6	2	$\bar{4}$	.85120	13	6	4	$\bar{1}$
1.5802	195	7	1	$\bar{1}$	1.1270	12	7	1	$\bar{5}$					
1.5761	15	4	2	0	1.0630	11	11	1	$\bar{2}$					

PDF # 440992, Wavelength = 1.5418 (A)

44-0992 Quality:
CAS Number:
Molecular Weight: 86.94
Volume[CD]: 517.78
Dx: 4.461 Dm: 4.490
S.G.: Fd3m (227)
Cell Parameters:
a 8.03 b c
α β γ
SS/FOM: F 8=7(0.119, 10)
I/Icor:
Rad: CuKa
Lambda: 1.5418
Filter:
d-sp: diffractometer

λ-Mn O2
Manganese Oxide
Ref: Hunter, J., J. Solid State Chem., 39, 142 (1981)

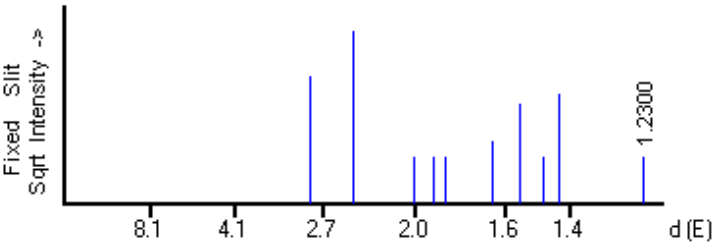


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
4.6400	100	1	1	1	2.0100	45	4	0	0	1.4200	26	4	4	0
2.4200	45	3	1	1	1.8400	6	3	3	1	1.3500	12	5	3	1
2.3100	8	2	2	2	1.5500	13	5	1	1					

PDF # 011146, Wavelength = 0.709 (A)

01-1146 (Deleted)
CAS Number:
Molecular Weight: 183.34
Volume[CD]: 524.00
Dx: 4.648 Dm: 4.580
S.G.: Fd3m (227)
Cell Parameters:
a 8.062 b c
α β γ
SS/FOM: F 8=15(0.041, 13)
I/Icor:
Rad: MoKa
Lambda: 0.709
Filter: ZrO2
d-sp:
Mineral Name:
Gahnite

Zn Al2 O4
Zinc Aluminum Oxide
Ref: Hanawalt et al., Anal. Chem., 10, 475 (1938)

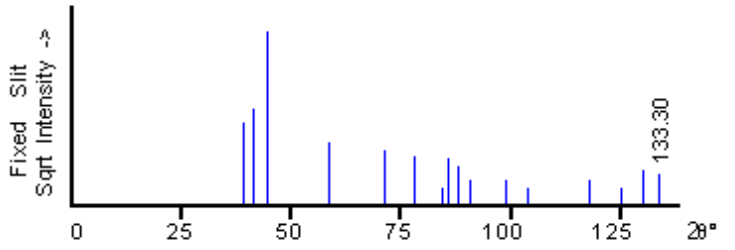


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.8500	53	2	2	0	1.8500	7	3	3	1	1.4300	40	4	4	0
2.4400	100	3	1	1	1.6500	13	4	2	2	1.2300	7	5	3	3
2.0200	7	4	0	0	1.5500	33	5	1	1					
1.9100	7				1.4800	7								

PDF # 451027, Wavelength = 1.54056 (A)

45-1027 Quality:
CAS Number: 7440-02-0
Molecular Weight: 58.70
Volume[CD]: 26.44
Dx: 7.372 Dm:
S.G.: P63/mmc (194)
Cell Parameters:
a 2.651 b c 4.343
α β γ
SS/FOM: F16=12(0.080, 16)
I/Icor:
Rad: CuKa1
Lambda: 1.54056
Filter:
d-sp: diffractometer

Ni
Nickel
Ref: Carturan, G et al., Materials Letters, 7, 47 (1988)

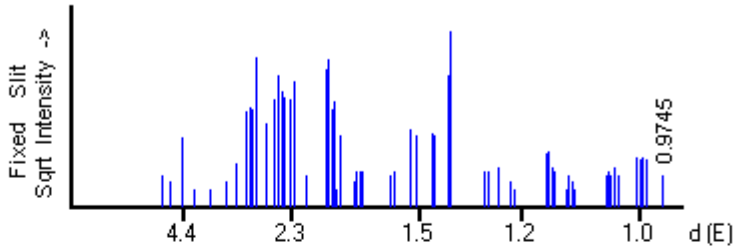


2θ	int-f	h	k	l	2θ	int-f	h	k	l	2θ	int-f	h	k	l
39.100	22	0	1	0	84.240	<1	2	0	0	117.93	2	2	0	3
41.530	30	0	0	2	85.790	7	1	1	2	125.16	<1	[2	1	0]
44.520	100	0	1	1	87.850	5	2	0	1	129.72	4	[2	1	1]
58.420	13	0	1	2	90.530	2	0	0	4	133.30	3	1	1	4
70.980	10	1	1	0	98.730	2	2	0	2					
78.000	8	1	0	3	103.57	<1	0	1	4					

PDF # 461131, Wavelength = 1.5418 (A)

46-1131 Quality:
CAS Number: 1344-28-1
Molecular Weight: 101.96
Volume[CD]: 741.62
Dx: 2.740 Dm:
S.G.: P$\bar{4}$m2 (115)
Cell Parameters:
a 5.599 b c 23.65
α β γ
SS/FOM: F30=5(0.090, 69)
I/Icor:
Rad: CuKa
Lambda: 1.5418
Filter:
d-sp: diffractometer

δ-Al2 O3
Aluminum Oxide
Ref: Repelin, Y., Husson, E., Mater. Res. Bull., 25, 611 (1990)

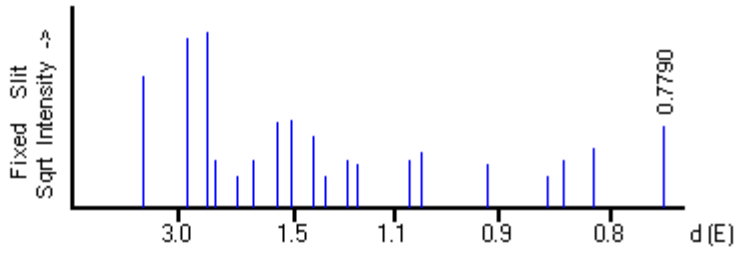


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
5.4666	3	0	1	1	1.9294	<1	[2	2	3]	1.1444	10	2	3	14
5.0633	2	0	1	2	1.9132	16	2	0	9	1.1401	5	0	4	12
4.5483	15	0	1	3	1.8178	2	0	3	3	1.1358	4	1	3	16
4.0733	<1	0	1	4	1.8060	4b	2	0	10	1.1128	1	0	5	2
3.6099	<1	0	1	5	1.7858	4	0	3	4	1.1108	1	0	4	13
3.2291	2	0	1	6	1.7710	4	1	3	0	1.1108	1	0	5	3
3.0495	6	1	1	5	1.7710	4	2	2	6	1.1072	3	2	4	10
2.8804	29	0	1	7	1.6284	3	1	2	11	1.1072	3	2	3	15
2.8115	32	0	2	0	1.6101	4	2	0	12	1.1008	2	0	5	4
2.7859	30	0	2	1	1.5381	19	2	3	2	1.0969	1	1	5	0
2.7280	71	0	2	2	1.5171	16	1	3	8	1.0477	3b	0	5	8
2.5901	22	1	1	7	1.5171	16	2	2	10	1.0477	3b	0	4	15
2.4925	37	1	2	1	1.4559	17	2	2	11	1.0442	4	1	5	7
2.4427	56	1	2	2	1.4454	16	0	2	14	1.0398	3b	3	3	14
2.4086	43	0	2	5	1.3996	56	0	4	0	1.0398	3b	2	5	0
2.3876	38	1	2	3	1.3959	90	0	4	1	1.0356	5	2	5	2
2.3730	34	1	0	9	1.3959	90	2	2	12	1.0300	3	3	4	9
2.3154	37	1	2	4	1.3911	100	0	4	2	1.0066	8	2	4	14
2.2794	50	0	2	6	1.2918	4	0	4	7	1.0066	8	2	5	6
2.1601	3	0	2	7	1.2837	4	2	2	14	.99960	7	1	4	16
2.0136	45	1	2	7	1.2589	5	1	4	7	.99650	8	1	5	10
2.0060	60	0	1	11	1.2589	5	2	3	11	.99280	7	0	5	11
1.9860	70	2	2	0	1.2265	2	3	3	7	.97450	3	3	4	12
1.9688	30	2	2	1	1.2171	<1	2	3	12					
1.9473	36	2	2	2	1.1506	9	2	4	8					

PDF # 471292, Wavelength = 1.54056 (A)

47-1292 Quality: I
CAS Number: 1344-28-1
Molecular Weight: 101.96
Volume[CD]: 501.47
Dx: 2.701 Dm: 3.550
S.G.: Fd3m (227)
Cell Parameters:
a 7.944 b c
α β γ
SS/FOM: F19=23(0.026, 32)
I/Icor:
Rad:
Lambda:
Filter:
d-sp:

σ-Al2 O3
Aluminum Oxide
Ref: Guse, W., Saalfeld, H., Neues Jahrb. Mineral., Monatsh., 1990, 217 (1990)



d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
4.5880	56	1	1	1	1.5290	24	5	1	1	.91700	6	7	5	1
2.8100	93	2	2	0	1.4050	16	4	4	0	.84700	3	6	6	4
2.3960	100	3	1	1	1.3430	3	5	3	1	.83300	7	9	3	1
2.2940	7	2	2	2	1.2560	7	6	2	0	.81100	11	8	4	4
1.9870	3	4	0	0	1.2120	6	5	3	3	.77900	21	8	6	2
1.8230	7	3	3	1	1.0620	7	6	4	2					
1.6220	23	4	2	2	1.0340	10	5	5	3					

PDF # 421120, Wavelength = 1.540598 (A)

42-1120 Quality: *

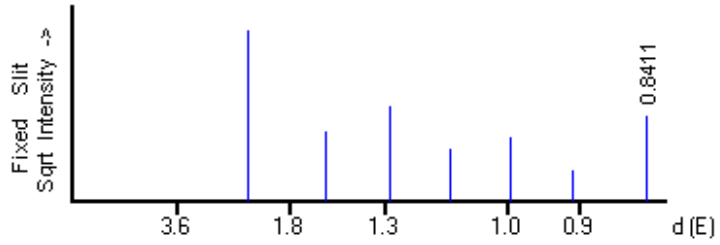
CAS Number:

Molecular Weight: 95.94
Volume[CD]: 31.17
Dx: 10.221 Dm:

S.G.: Im3m (229)
Cell Parameters:
a 3.147 b c
α β γ

SS/FOM: F 7=80(.0126, 7)
I/Icor: 7.379
Rad: CuKa1
Lambda: 1.5405988
Filter: Graph
d-sp: diffractometer

Mo
Molybdenum
Ref: Schreiner, W., Intelligent Controls Inc., Amawalk, NY, USA, ICDD Grant-in-Aid, (1991)



d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.2247	100	1	1	0	1.1129	9	2	2	0	.84109	24	3	2	1
1.5738	16	2	0	0	.99533	14	3	1	0					
1.2846	31	2	1	1	.90847	3	2	2	2					

PDF # 461215, Wavelength = 1.5418 (A)

46-1215 Quality: I

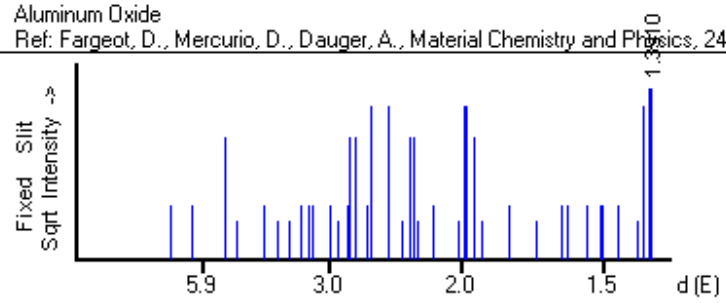
CAS Number:

Molecular Weight: 101.96
Volume[CD]: 739.23
Dx: Dm:

S.G.: P222 (16)
Cell Parameters:
a 7.934 b 7.956 c 11.71
α β γ

SS/FOM: F30=6(0.043,120)
I/Icor:
Rad: CuKa
Lambda: 1.5418
Filter:
d-sp: Guinier

δ*-Al2 O3
Aluminum Oxide
Ref: Fargeot, D., Mercurio, D., Dauger, A., Material Chemistry and Physics, 24, 299 (1990)



d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
7.9700	10	0	1	0	2.8080	10	2	2	0	1.9830	80	4	0	0
7.9700	10	1	0	0	2.7870	50	0	2	3	1.9510	50	0	0	6
6.5500	10	0	1	1	2.7870	50	2	0	3	1.9070	5	1	3	4
6.5500	10	1	0	1	2.7310	50	2	2	1	1.9070	5	3	1	4
5.0600	50	1	1	1	2.6270	10	1	2	3	1.7990	10	2	2	5
4.7160	5	0	1	2	2.6270	10	2	1	3	1.7010	5	2	4	2
4.7160	5	1	0	2	2.5960	80	1	1	4	1.7010	5	4	2	2
4.0540	10	1	1	2	2.4570	80	1	3	1	1.6150	10	1	4	4
3.7540	5	0	2	1	2.4570	80	3	1	1	1.6150	10	4	1	4
3.7540	5	2	0	1	2.3530	5	0	2	4	1.6020	10	1	1	7
3.5500	5	1	2	0	2.3530	5	2	0	4	1.6020	10	2	2	6
3.5500	5	2	1	0	2.3080	50	1	3	2	1.5420	10	1	5	1
3.3940	10	1	2	1	2.3080	50	3	1	2	1.5420	10	5	1	1
3.3940	10	2	1	1	2.2800	50	2	2	3	1.5080	10	1	5	2
3.2820	10	0	2	2	2.2560	5	1	2	4	1.5030	10	5	1	2
3.2820	10	2	0	2	2.2560	5	2	1	4	1.4630	10	3	3	5
3.2100	10	1	1	3	2.1620	10	1	1	5	1.4170	5	1	1	8
3.0060	10	1	2	2	2.0190	5	0	2	5	1.4050	80	4	4	0
3.0060	10	2	1	2	2.0190	5	2	0	5	1.3920	100	0	4	6
2.9230	5	0	0	4	1.9900	80	0	4	0	1.3910	100	4	0	6

PDF # 011205, Wavelength = 0.709 (A)

01-1205 (Deleted)

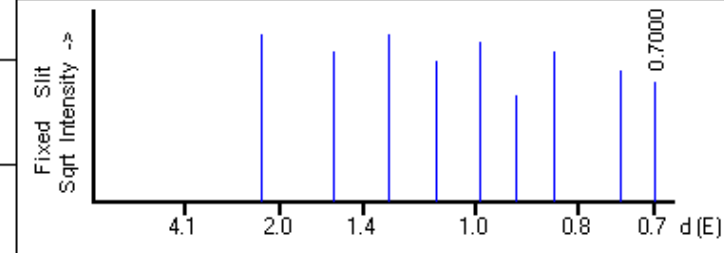
CAS Number:

Molecular Weight: 95.94
Volume[CD]: 31.08
Dx: 10.252 Dm: 10.210

S.G.: Im3m (229)
Cell Parameters:
a 3.144 b c
α β γ

SS/FOM: F 9=9(0.105, 10)
I/Icor:
Rad: MoKa
Lambda: 0.709
Filter:
d-sp:

Mo
Molybdenum
Ref: Davey, Phys. Rev., 25, 753 (1925)

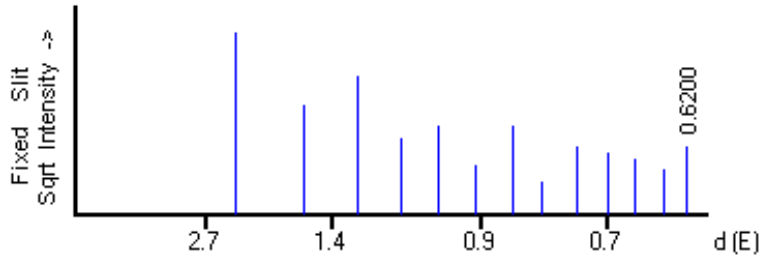


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.2300	100	1	1	0	1.1100	70	2	2	0	.84000	80	3	2	1
1.5700	80	2	0	0	.99000	90	3	1	0	.74000	60	3	3	0
1.2800	100	2	1	1	.91000	40	2	2	2	.70000	50	4	2	0

PDF # 011207, Wavelength = 0.709 (A)

01-1207 (Deleted)
CAS Number:
Molecular Weight: 95.94
Volume[CD]: 30.96
Dx: 10.292 Dm: 10.200
S.G.: Im3m (229)
Cell Parameters:
a 3.140 b c
α β γ
SS/FOM: F12=9(0.113, 12)
I/Icor:
Rad: MoKa
Lambda: 0.709
Filter: ZrO2
d-sp:

Mo
Molybdenum
Ref: Hanawalt et al., Anal. Chem., 10, 475 (1938)

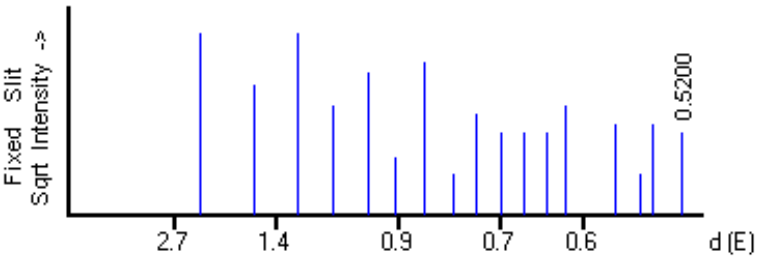


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.2200	100	1	1	0	.91000	7	2	2	2	.67000	9	3	3	2
1.5700	36	2	0	0	.84000	23	3	2	1	.64000	6	4	2	2
1.2800	57	2	1	1	.79000	3	4	0	0	.62000	14			
1.1100	17	2	2	0	.74000	14	3	3	0					
1.0000	23	3	1	0	.70000	11	4	2	0					

PDF # 011208, Wavelength = 0.709 (A)

01-1208 (Deleted)
CAS Number:
Molecular Weight: 95.94
Volume[CD]: 31.05
Dx: 10.262 Dm: 10.160
S.G.: Im3m (229)
Cell Parameters:
a 3.143 b c
α β γ
SS/FOM: F14=6(0.150, 15)
I/Icor:
Rad: MoKa
Lambda: 0.709
Filter:
d-sp:

Mo
Molybdenum
Ref: Hull, Phys. Rev., 17, 571 (1921)

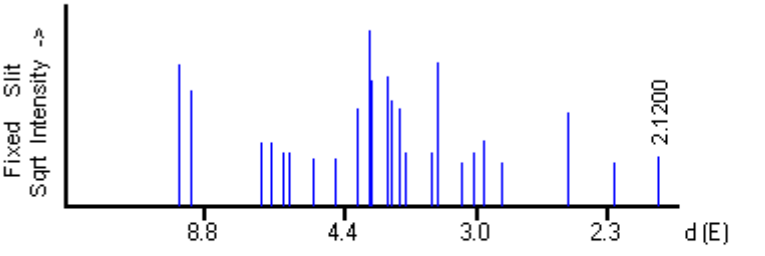


d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
2.2200	100	1	1	0	.84000	70	3	2	1	.62000	35	5	1	0
1.5700	50	2	0	0	.78000	5	4	0	0	.57000	25			
1.2800	100	2	1	1	.74000	30	3	3	0	.55000	5			
1.1100	35	2	2	0	.70000	20	4	2	0	.54000	25	5	3	0
.99000	60	3	1	0	.67000	20	3	3	2	.52000	20			
.91000	10	2	2	2	.64000	20	4	2	2					

PDF # 470718, Wavelength = 1.5418 (A)

47-0718 Quality: O
CAS Number:
Molecular Weight: 60.08
Volume[CD]:
Dx: Dm:
S.G.:
Cell Parameters:
a b c
α β γ
SS/FOM: F = (,)
I/Icor:
Rad: CuKa
Lambda: 1.5418
Filter:
d-sp: diffractometer

Si O2
Silicon Oxide
Ref: Young, D., 4,325,929, U.S. Patent, (1982)



d(A)	int-f	h	k	l	d(A)	int-f	h	k	l	d(A)	int-f	h	k	l
10.900	64				4.2300	31				3.3300	66			
9.8300	42				4.0600	100				3.1300	6			
6.2800	13				4.0200	51				3.0300	9			
5.9500	13				3.8300	54				2.9700	14			
5.6600	9				3.7900	35				2.8400	6			
5.5200	9				3.7000	30				2.4800	28			
4.9600	7				3.6300	9				2.2800	6			
4.5800	7				3.3800	9				2.1200	8			