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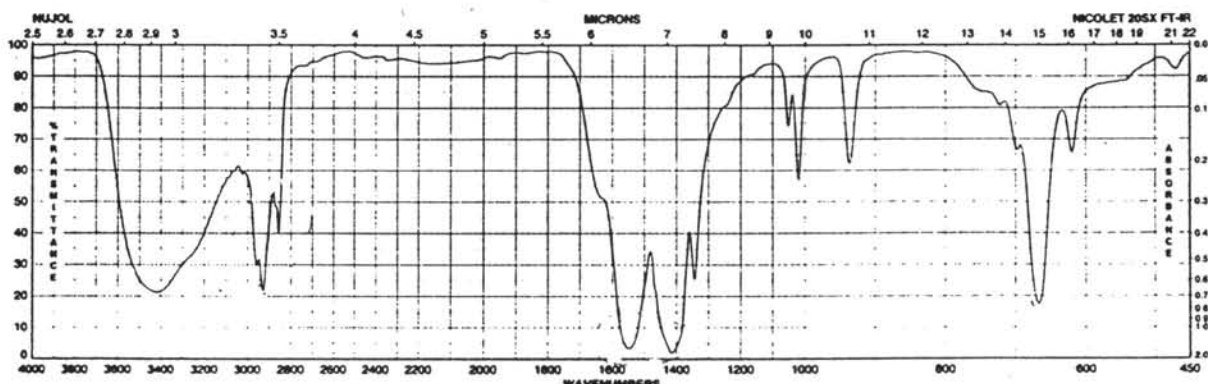
Zhenfang, Tang., Xingui, Tang.(2003) Structural, dielectric and optical properties of highly oriented lead zirconate thin films prepared by sol-gel process. Materials Chemistry and Physics, 80, 294-298.

APPENDICES

Appendix A The FTIR standard patterns of starting materials.

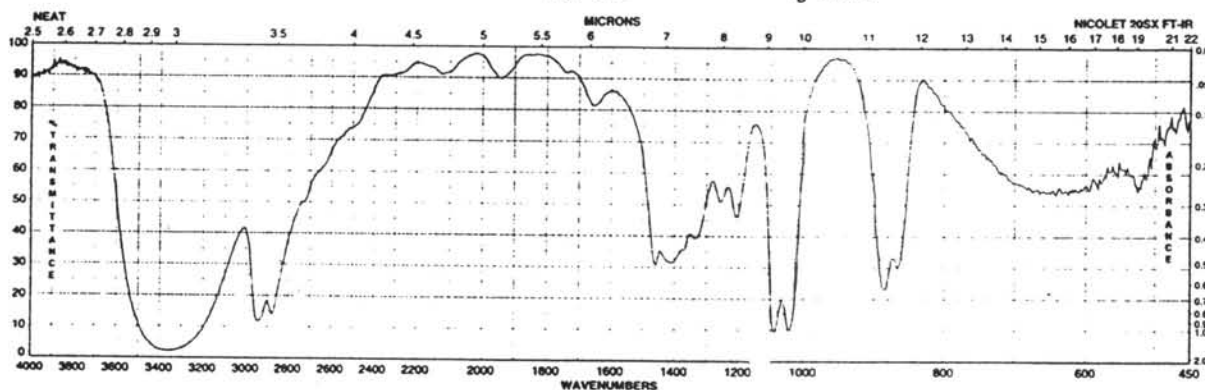
Lead acetate trihydrate

Aldrich 31,651-2 CAS [6080-56-4] $C_2H_4O_2$
Lead(II) acetate trihydrate, 99.999% FW 379.33



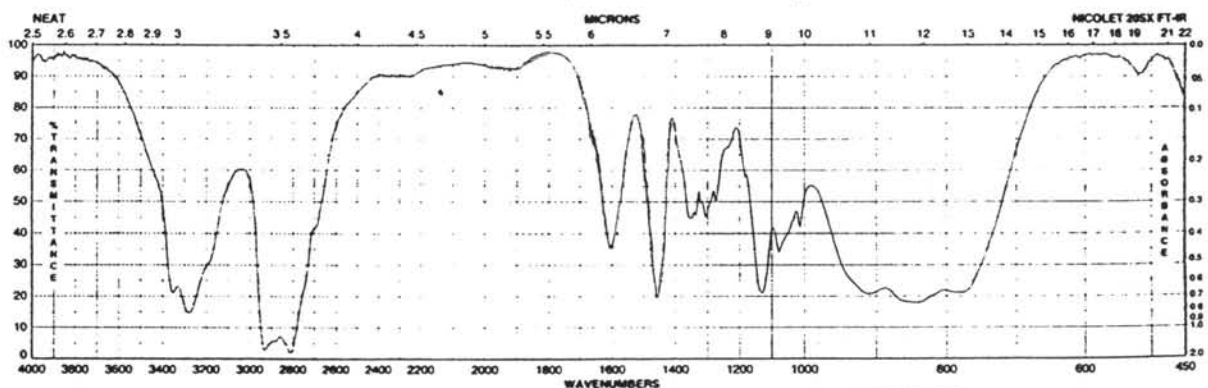
Ethylene glycol

Aldrich 10,246-6 CAS [107-21-1] $C_2H_6O_2$ bp 196 – 198 °C Fp >230 °F
Ethylene glycol, 99+% FW 62.07 mp -13 °C d 1.113 VP-FT-IR: 3, 188B
n_D²⁰ 1.4310



Triethylenetetramine

Aldrich 13,209-8 CAS [112-24-3] $C_6H_{18}N_4$ bp 266 – 267 °C Fp 290 °F
Triethylenetetramine, tech., 60% FW 146.24 mp 12 °C d 0.982 FT-NMR: 1, 501C
n_D²⁰ 1.4971 VP-FT-IR: 3, 398B



Appendix B The XRD standard peak patterns of synthesis lead glycolate, lead titanate, lead zirconate, and lead zirconate titanate.

38-1477					Wavelength= 1.5405981					
PbO	2 θ	Int	h	k	l	2 θ	Int	h	k	l
Lead Oxide	15.017	4	0	1	0	90.704	1	2	5	0
	22.111	1	1	1	0					
	29.079	100	1	1	1					
Massicot	30.316	24	0	2	0					
Rad.: CuK α 1 λ : 1.540598 Filter: Graph Mono d-sp: Diff.	32.594	23	2	0	0					
Cut off: 17.7 Int.: Diffract. I/cor.:	36.067	<1	2	1	0					
Ref: McMurdie, H et al., Powder Diffraction, 2, 46 (1987)	37.822	17	2	0	1					
	39.515	1	1	2	1					
	40.929	<1	0	1	2					
	45.120	13	2	2	0					
	46.192	2	0	3	0					
Sys.: Orthorhombic S.G.: Pcam (57)	49.230	12	0	2	2					
a: 5.4903(4) b: 5.8920(4) c: 4.7520(4) A: 0.9318 C: 0.8065	50.783	13	2	0	2					
α :	52.305	<1	3	1	0					
β :	53.105	16	1	3	1					
γ :	56.025	15	3	1	1					
Z: 4 mp:	57.641	<1	2	3	0					
Ref: Ibid.	60.301	11	2	2	2					
	61.174	<1	0	3	2					
Dx: 9.644 Dm: SS/FOM: F ₃₀ = 88 (.0062, 55)	63.062	12	0	4	0					
	66.352	1	3	1	2					
Color: Orange-yellow	68.280	1	4	0	0					
Peak height intensity. The mean temperature of data collection was 25.2 C. The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ, USA. CAS #: 1317-36-8. The pattern is complicated by the presence of a small percentage of the red (tetragonal) form. Five weak reflections of the red form appear at d=3.1130, 2.8097, 2.5091, 1.8728 and 1.6780. References to other early patterns will be found in Swanson and Fuyat (4). $\sigma(I_{\text{obs}}) = \pm 0.01$. The orthorhombic phase of PbO is stable above 500 C, the red form (litharge, tetragonal) is stable below 500 C (3). The crystal structure of the yellow PbO was determined by Leciejewicz (1) and Kay (2) by means of neutron diffraction. O Pb type. Also called: lead monoxide. Silver, fluorophlogopite used as an internal stands. PSC: oP8. To replace 5-570 (4) and validated by calculated pattern. Mwt: 223.20. Volume[CD]: 153.72.	68.840	1	1	4	1					
	69.456	<1	1	2	3					
	71.057	1	2	3	2					
	72.797	2	2	4	0					
	73.414	3	3	3	1					
	75.944	2	0	4	2					
	76.489	2	4	2	0					
	79.617	4	1	3	3					
	80.825	2	0	0	4					
	82.033	3	3	1	3					
	85.090	2	1	1	4					
	86.931	2	1	5	1					
	88.693	3	4	2	2					
	89.909	1	2	0	4					



40-0099

Wavelength= 1.5418

PbTiO₃

Lead Titanium Oxide

2 θ	Int	h	k	l
22.451	35	1	0	0
31.951	100	1	1	0
39.398	40	1	1	1
45.827	35	2	0	0
51.608	10	2	1	0
56.985	35	2	1	1

Rad.: CuK α λ : 1.5418 Filter: Ni Beta d-sp:

Cut off: Int.: I/cor.:

Ref: Yamaguchi, O et al., J. Am. Ceram. Soc., 69, C256 (1986)

Sys.: Cubic

S.G.:

a: 3.961 b: c: A: C:

 α : β : γ : Z: mp:

Ref: Ibid.

Dx: Dm: SS/FOM: $F_6 = 79 (.0127, 6)$

Pattern taken at 680 C. Made using Pb (O C3 H7)2 and Ti (O C3 H7)4. C phase. Reflections somewhat broad.
Perovskite, Ca O3 Ti type. Mwt: 303.10. Volume[CD]: 62.15.



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70-0746		Wavelength= 1.54060									
PbTiO ₃		2 θ	Int	h	k	l	2 θ	Int	h	k	l
Lead Titanium Oxide		21.363	242	0	0	1	84.112	44	2	2	2
		22.754	361	1	0	0	85.966	19	2	0	3
		31.409	999*	1	0	1	88.581	15	3	0	2
		32.397	451	1	1	0					
		39.136	336	1	1	1					
		43.517	109	0	0	2					
		46.472	243	2	0	0					
		49.658	108	1	0	2					
		51.684	77	2	0	1					
		52.346	67	2	1	0					
		55.283	172	1	1	2					
		57.168	306	2	1	1					
		65.551	105	2	0	2					
		67.565	12	0	0	3					
		67.826	63	2	2	0					
		70.363	64	2	1	2					
		72.019	26	2	2	1					
		72.313	67	1	0	3					
		72.567	40	3	0	0					
		76.650	55	3	0	1					
		76.939	36	1	1	3					
		77.187	61	3	1	0					
		81.196	51	3	1	1					
Rad.: CuK α 1 λ : 1.54060 Filter:		d-sp: Calculated									
Cut off: 17.7 Int.: Calculated		I/cor.: 11.74									
Ref: Calculated from ICSD using POWD-12+., (1997)											
Ref: Glazer, A.M., Mabud, S.A., Acta Crystallogr., Sec. B, 34, 1065 (1978)											
Sys.: Tetragonal		S.G.: P4mm (99)									
a: 3.905	b:	c: 4.156	A:	C: 1.0643							
α :	β :	γ :	Z: 1	mp:							
Ref: Ibid.											
Dx: 7.942	Dm:	ICSD #: 001612									
Peak height intensity. R-factor: 0.045. PSC: TP5. Mwt: 303.10. Volume[CD]: 63.37.											

70-1016		Wavelength= 1.54060												C								
PbTi3O7													2 θ	Int	h	k	l	2 θ	Int	h	k	l
Lead Titanium Oxide													8.330	879	1	0	0	35.883	30	3	1	1
													13.594	619	0	0	1	36.330	267	0	1	2
													14.899	214	1	0	1	36.330	267	1	1	2
													16.963	373	1	0	1	38.202	271	1	1	2
													20.002	55	2	0	1	38.384	209	2	1	2
Rad.: CuK α 1: 1.54060 Filter: d-sp: Calculated													23.088	257	2	0	1	38.384	209	4	0	1
Cut off: 17.7 Int.: Calculated I/cor.: 2.65													24.799	34	1	1	0	38.690	49	3	1	1
Ref: Calculated from ICSD using POWD-12++, (1997)													25.168	305	3	0	0	40.241	92	3	0	2
Ref: Kato, K., Kawada, I., Muramatsu, K., Acta Crystallogr., Sec. B, 30, 1634 (1974)													26.889	91	3	0	1	40.648	52	4	0	2
													27.087	18	0	1	1	41.222	46	1	0	3
													27.466	445	1	0	2	41.448	129	4	1	0
Sys.: Monoclinic S.G.: P2 ₁ /m (11)													27.783	582	1	1	1	41.593	151	0	0	3
a: 10.718(5) b: 3.812(1) c: 6.577(7) A: 2.8116 C: 1.7253													28.820	775	2	1	0	41.901	99	2	1	2
													28.976	671	1	1	1	42.156	111	4	1	1
α : β : 98.270(7) γ : Z: 2 mp:													29.830	401	1	0	2	42.156	111	3	1	2
Ref: Ibid.													30.057	46	2	0	2	42.584	8	5	0	0
													30.434	351	3	0	1	42.862	116	5	0	1
													30.906	999*	2	1	1	43.740	40	1	0	3
Dx: 5.781 Dm: 5.782 ICSD #: 002104													33.046	234	2	1	1	45.432	61	4	1	1
													33.776	330	4	0	0	45.778	49	3	0	3
													34.313	32	2	0	2	46.879	5	5	0	1
Peak height intensity. R-factor: 0.083. PSC: mP22. Mwt: 462.90. Volume[CD]: 265.92.													34.646	404	4	0	1	47.026	11	3	1	2
													34.646	404	3	0	2	47.188	54	4	0	2

2 θ	Int	h	k	l	2 θ	Int	h	k	l	2 θ	Int	h	k	l	2 θ	Int	h	k	l
47.386	54	4	1	2	59.698	98	4	2	0	72.563	11	0	0	5	82.215	65	4	2	4
47.468	47	2	0	3	60.046	16	2	2	2	72.828	22	6	2	1	82.503	66	2	3	2
47.675	381	5	0	2	60.264	145	4	2	1	72.928	20	6	2	0	82.503	66	6	2	3
47.675	381	0	2	0	60.264	145	3	2	2	73.100	23	8	0	2	82.696	37	7	0	3
47.895	139	1	1	3	60.455	127	5	1	2	73.100	23	6	0	4	82.696	37	2	1	5
48.225	17	0	1	3	60.678	47	7	0	1	73.634	45	3	2	3	82.963	17	9	0	2
48.487	23	1	2	0	61.111	22	7	0	0	73.793	34	6	0	3	82.963	17	6	2	2
49.110	140	5	1	0	61.256	16	6	1	1	73.793	34	3	0	5	83.475	20	7	2	2
49.180	157	2	1	3	61.532	104	5	1	3	74.670	8	1	0	5	83.698	29	8	1	3
49.358	128	5	1	1	62.129	86	2	1	4	75.240	17	8	1	1	83.830	31	5	1	4
49.810	43	0	2	1	62.476	90	4	0	4	75.240	17	1	3	0	84.479	12	4	3	0
50.147	57	1	1	3	62.798	38	6	0	3	75.924	45	8	1	0	84.617	21	7	2	1
50.229	40	1	2	1	62.798	38	4	2	1	76.063	27	6	2	2	84.780	15	7	1	4
50.229	40	4	0	3	63.331	2	6	0	2	76.356	64	0	3	1	84.780	15	2	3	2
50.963	31	1	2	1	63.910	70	7	0	2	76.356	64	6	2	1	84.970	15	4	3	1
51.545	31	6	0	1	63.910	70	1	1	4	76.621	62	5	2	3	84.970	15	3	3	2
51.666	40	6	0	0	64.108	69	3	2	2	76.621	62	1	3	1	85.222	19	5	2	3
51.992	27	3	1	3	64.246	28	3	1	4	76.990	73	2	1	5	85.390	11	9	1	1
52.192	17	2	2	1	64.402	28	4	2	2	76.990	73	0	2	4	85.532	23	5	1	5
52.524	78	3	0	3	64.818	20	1	2	3	77.203	87	4	1	4	85.812	15	9	0	1
52.996	116	5	1	1	65.089	61	0	2	3	77.203	87	1	3	1	85.938	11	3	2	4
53.278	89	4	1	2	65.089	61	7	0	1	77.861	30	8	1	2	86.087	7	6	0	5
53.534	213	2	1	3	65.797	20	5	0	3	77.861	30	6	1	4	86.337	19	9	1	0
53.700	184	5	1	2	65.797	20	5	2	0	77.995	23	2	0	5					
54.662	60	3	2	0	66.026	50	5	2	1	78.189	56	2	3	1					
55.422	32	6	0	2	66.578	14	3	0	4	78.613	17	6	1	3					
55.583	43	3	2	1	66.683	15	1	2	3	78.613	17	3	1	5					
55.767	113	6	0	1	67.148	36	2	1	4	78.867	34	4	2	3					
55.901	145	1	0	4	67.638	8	4	1	4	79.075	23	3	2	4					
55.901	145	1	2	2	67.947	7	6	1	3	79.075	23	5	0	4					
56.059	64	5	0	3	68.237	25	3	2	3	79.344	19	2	3	1					
56.167	35	4	1	3	68.458	27	6	1	2	79.472	18	1	1	5					
56.511	82	0	0	4	68.984	11	7	1	2	79.884	27	8	1	1					
56.692	60	2	0	4	69.333	25	4	2	2	80.017	16	7	0	4					
57.300	235	1	2	2	69.553	17	2	2	3	80.616	22	7	2	1					
57.300	235	6	1	1	69.695	14	5	2	2	80.616	22	9	0	1					
57.413	139	2	2	2	70.437	22	7	0	3	81.000	18	3	3	1					
57.413	139	6	1	0	70.834	21	5	1	3	81.000	18	7	2	0					
57.619	102	3	2	1	71.042	11	8	0	0	81.240	27	0	3	2					
58.213	3	3	1	3	71.710	13	1	0	5	81.240	27	1	3	2					
58.571	13	1	0	4	71.834	7	4	2	3	81.482	22	4	1	5					
58.684	39	4	0	3	72.310	6	4	0	4	81.631	5	9	0	0					
58.924	19	3	0	4	72.433	13	7	0	2	81.758	8	2	2	4					



71-0561

Wavelength= 1.54060

C

Pb3O4

Lead Oxide

Rad.: CuK α 1 λ : 1.54060 Filter: d-sp: Calculated

Cut off: 17.7 Int.: Calculated I/cor.: 13.09

Ref: Calculated from ICSD using POWD-12++, (1997)

Ref: Gavarrri, J.R., Weigel, D., J. Solid State Chem., 13, 252 (1975)

Sys.: Tetragonal

S.G.: P4 $_2$ /mbc (135)

a: 8.811 b: c: 6.563 A: C: 0.7449

 α : β : γ : Z: 4 mp:

Ref: Ibid.

Dx: 8.938

Dm:

ICSD #: 004106

Peak height intensity, R-factor: 0.060, PSC: tP28, Mwt: 685.60, Volume[Å^3]: 509.51

2θ	Int	h	k	l	2θ	Int	h	k	l
14.204	135	1	1	0	46.285	25	2	0	3
20.140	16	2	0	0	47.499	167	2	1	3
22.546	10	2	1	0	48.185	9	4	2	1
24.314	28	2	0	1	49.818	205	4	0	2
26.361	999*	2	1	1	50.955	10	4	1	2
27.153	53	0	0	2	52.074	216	3	3	2
28.633	128	2	2	0	52.947	20	5	1	0
30.771	365	1	1	2	53.822	10	4	3	1
32.098	468	3	1	0	54.263	12	4	2	2
34.040	248	2	0	2	54.900	7	5	1	1
34.957	4	3	1	1	56.001	55	0	0	4
35.574	2	2	1	2	56.172	30	5	2	0
36.748	21	3	2	0	56.405	12	3	2	3
39.310	39	3	2	1	58.052	103	5	2	1
39.870	51	2	2	2	58.052	103	1	1	4
40.938	15	4	0	0	59.280	41	4	4	0
42.257	1	4	1	0	59.493	24	4	3	2
42.529	1	3	1	2	59.493	24	4	0	3
43.292	6	4	0	1	60.130	2	2	0	4
43.544	8	3	3	0	60.505	74	5	1	2
44.554	89	4	1	1	60.505	74	4	1	3
46.030	98	4	2	0	61.135	2	2	1	4
46.285	25	3	2	2	61.297	16	5	3	0

2θ	Int	h	k	l	2θ	Int	h	k	l
63.082	12	5	3	1	82.791	51	5	4	3
63.276	49	6	0	0	83.489	32	7	3	0
63.492	26	5	2	2	83.489	32	3	2	5
63.492	26	4	2	3	84.554	42	6	4	2
64.095	18	2	2	4	85.075	3	7	3	1
64.252	13	6	1	0	85.433	7	7	2	2
65.030	4	6	0	1	85.985	20	4	4	4
66.026	97	6	1	1	86.127	5	6	5	0
66.026	97	3	1	4	86.180	11	4	0	5
67.136	3	6	2	0	86.180	11	6	3	3
68.083	2	5	4	0	87.057	8	4	1	5
68.281	18	5	3	2	87.740	14	6	5	1
68.281	18	4	3	3	87.740	14	5	3	4
68.872	4	6	2	1	88.757	4	8	0	0
68.872	4	3	2	4	89.492	26	6	0	4
69.231	3	5	1	3	89.492	26	0	0	6
69.775	24	5	4	1	89.817	16	7	3	2
70.154	2	6	0	2					
71.082	6	6	1	2					
71.663	4	4	0	4					
72.017	46	5	2	3					
72.584	1	4	1	4					
73.499	3	6	3	1					
73.499	3	3	3	4					
73.839	27	6	2	2					
74.748	4	5	4	2					
75.318	33	4	2	4					
75.519	18	2	0	5					
76.422	33	5	5	0					
76.422	33	2	1	5					
77.987	1	7	1	1					
78.163	1	6	4	0					
78.362	2	6	3	2					
78.362	2	6	0	3					
79.057	7	7	2	0					
79.255	10	6	1	3					
79.772	6	6	4	1					
79.772	6	4	3	4					
80.692	11	7	2	1					
80.692	11	5	1	4					
80.859	6	3	1	5					
81.918	1	6	2	3					
82.791	51	7	1	2					



PDF#05-0561: QM=Indexed(I); d=(Unknown); I=Diffractometer												PDF Card	
Litharge, syn												(Litharge)	
Pb O													
Radiation=CuKα1				Lambda=1.5405				Filter=Ni					
Calibration=				2θ=17.660-113.704				I/c(RIR)=					
Ref: Swanson, Fuyat.													
Natl. Bur. Stand. (U.S.), Circ. 539, vII p30 (1953)												CAS#:1317-36-8	
Tetragonal - Powder Diffraction, P4/nmm (129)								Z=2		mp=			
CELL: 3.9729 x 3.9729 x 5.0217 <90.0 x 90.0 x 90.0>												P.S=IP4 (O Pb)	
Density(c)=9.354		Density(m)=10.02A		Mwt=223.20		Vol=79.26		F(27)=25.9(0.023,46/0)					
Ref: Ibid.													
NOTE: Crystal system refined in 1975. Sample from National Lead Company. Spectroscopic analysis: <0.01% Bi, Cu, Fe, Si; <0.001% Ca, Mg. Pattern taken at 27 C. Polymorph: massicot (tetragonal). Validated by calculated pattern. See ICSD 62842 (PDF 85-1289); See ICSD 26596 (PDF 85-711); See ICSD 62840 (PDF 85-1287); See ICSD 62841 (PDF 85-1288); See ICSD 62842 (PDF 85-1289); See ICSD 62843 (PDF 85-1290).													
Color: Violet-red													
Strong Lines: 3.12/X 2.81/6 1.87/4 1.68/2 2.51/2 1.54/1 1.99/1 1.56/1 5.02/1 1.41/1													
27 Lines, Wavelength to Compute Theta = 1.54056A(Cu), I%-Type = (Unknown)													
#	d(Å)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	#	d(Å)	I(f)	(h k l)	2-Theta	Theta	1/(2d)
1	5.0180	5.0	(0 0 1)	17.660	8.830	0.0996	15	1.2260	4.0	(2 2 2)	77.848	38.924	0.4078
2	3.1150	100.0	(1 0 1)	28.633	14.317	0.1605	16	1.2190	5.0	(3 1 1)	78.380	39.190	0.4102
3	2.8090	62.0	(1 1 0)	31.831	15.915	0.1780	17	1.1977	0.0	(1 0 4)	80.052	40.026	0.4175
4	2.5100	18.0	(0 0 2)	35.743	17.872	0.1992	18	1.1462	2.0	(1 1 4)	84.448	42.224	0.4362
5	2.1240	1.0	(1 0 2)	42.527	21.263	0.2354	19	1.1232	2.0	(3 1 2)	86.596	43.298	0.4452
6	1.9880	8.0	(2 0 0)	45.594	22.797	0.2515	20	1.0768	3.0	(3 2 1)	91.342	45.671	0.4643
7	1.8720	37.0	(1 1 2)	48.595	24.297	0.2671	21	1.0610	2.0	(2 0 4)	93.103	46.552	0.4713
8	1.6750	24.0	(2 1 1)	54.757	27.379	0.2985	22	1.0386	0.0	(3 0 3)	95.745	47.872	0.4814
9	1.5580	6.0	(2 0 2)	59.261	29.630	0.3209	23	1.0254	0.0	(2 1 4)	97.389	48.694	0.4876
10	1.5420	11.0	(1 0 3)	59.938	29.969	0.3243	24	0.9738	1.0	(1 0 5)	104.559	52.279	0.5135
11	1.4380	2.0	(1 1 3)	64.777	32.389	0.3477	25	0.9462	1.0	(4 1 1)	108.992	54.496	0.5284
12	1.4050	5.0	(2 2 0)	66.493	33.246	0.3559	26	0.9365	3.0	(3 3 0)	110.674	55.337	0.5339
13	1.2820	2.0	(3 0 1)	73.861	36.930	0.3900	27	0.9200	3.0	(3 2 3)	113.704	56.852	0.5435
14	1.2560	3.0	(3 1 0)	75.654	37.827	0.3981							

PDF#14-0031: QM=Doubtful(O); d=Other/Unknown(90.0mm); I=Film/Visual													PDF Card	
Lead Titanium Zirconium Oxide														
Pb2 (Ti , Zr) O3														
Radiation=FeKa					Lambda=1.9373					Filter=Mn				
Calibration=					2T=21.873-102.167					I/c(RIR)=				
Ref: Barnes, Hurley, Chem. Dept., Group Research Centre, Joseph Lucas Ltd., The Radleys, Marston Green, Birmingham, England,...														
Private Communication														
Tetragonal - Powder Diffraction,														
CELL: 4.04 x 4.04 x 4.129 <90.0 x 90.0 x 90.0>														
Density(c)=12.574 Density(m)=9.21A Mwt=510.30 Vol=67.39 Z= mp=														
Ref: Ibid.														
P.S.=170 (?)														
F(19)=2.7(0.216,33/2)														
NOTE: O assigned because average \$VD,\$GU is 0.216.														
Color: Light yellow														
Strong Lines: 2.96/X 1.65/7 1.67/3 1.08/4 1.44/3 1.28/3 1.09/3 2.02/2 1.43/2 1.30/2														
21 Lines, Wavelength to Compute Theta = 1.54056A(Cu), I%-Type = (Unknown)														
#	d(A)	I(I)	(h k l)	2-Theta	Theta	1/(2d)	#	d(A)	I(I)	(h k l)	2-Theta	Theta	1/(2d)	
1	4.0600	5.0	(1 0 0)	21.873	10.937	0.1232	12	1.3000	20.0	(1 0 3)	72.673	36.336	0.3846	
2	2.9560	100.0		30.209	15.105	0.1691	13	1.2780	30.0	(3 1 0)	74.130	37.065	0.3912	
3	2.3380	15.0	(1 1 1)	38.472	19.236	0.2139	14	1.2360	5.0	(1 1 3)	77.101	38.550	0.4045	
4	2.0480	10.0	(0 0 2)	44.186	22.093	0.2441	15	1.2180	10.0	(3 1 1)	78.457	39.228	0.4105	
5	2.0170	20.0	(2 0 0)	44.902	22.451	0.2479	16	1.1720	20.0	(2 2 2)	82.179	41.089	0.4266	
6	1.8180	5.0	(2 0 1)	50.136	25.068	0.2750	17	1.0940	30.0	(2 1 3)	89.513	44.756	0.4570	
7	1.6700	30.0	(1 1 2)	54.935	27.468	0.2994	18	1.0830	40.0	(3 2 1)	90.673	45.336	0.4617	
8	1.6500	70.0	(2 1 1)	55.658	27.829	0.3030	19	1.0100	10.0	(4 0 0)	99.397	49.699	0.4950	
9	1.4410	30.0	(2 0 2)	64.626	32.313	0.3470	20	1.0000	10.0	(1 0 4)	100.758	50.379	0.5000	
10	1.4280	20.0	(2 2 0)	65.287	32.644	0.3501	21	0.9900	10.0		102.167	51.083	0.5051	
11	1.3560	10.0	(2 1 2)	69.229	34.615	0.3687								

PDF#26-0142: QM=Blank(B); d=(Unknown); I=Diffraction											PDF Card		
Lead Titanium Oxide													
Pb2 Ti2 O6													
Radiation=CuKa1			Lambda=1.5406			Filter=							
Calibration=			2T=14.605-69.229			I/c(RIR)=							
Ref: Martin.													
Phys. Chem. Glasses, v6 p143 (1965)													
Cubic - Powder Diffraction, Fd-3m (227)						Z=8		mp=					
CELL: 10.4 x 10.4 x 10.4 <90.0 x 90.0 x 90.0>													
Density(c)=7.160			Density(m)=7.57A		Mwt=606.20		Vol=1124.86		F(13)=8.3(0.087,18/0)				
Ref: Ibid.													
NOTE: Metastable modification. Pyrochlore type, oxygen deficient. To replace 20-601.													
Color: Yellow													
Strong Lines: 3.02/X 2.61/6 1.84/6 3.15/5 1.57/5 2.39/4 6.06/3 2.01/2 1.76/2 1.50/1													
13 Lines, Wavelength to Compute Theta = 1.54056A(Cu), I%-Type = (Unknown)													
#	d(A)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	#	d(A)	I(f)	(h k l)	2-Theta	Theta	1/(2d)
1	6.0600	25.0	(1 1 1)	14.605	7.303	0.0825	8	1.7580	20.0	(5 3 1)	51.973	25.986	0.2844
2	3.1500	50.0	(3 1 1)	28.309	14.154	0.1587	9	1.5880	8.0	(5 3 3)	58.033	29.017	0.3149
3	3.0200	100.0	(2 2 2)	29.554	14.777	0.1656	10	1.5700	45.0	(6 2 2)	58.763	29.382	0.3185
4	2.6100	55.0	(4 0 0)	34.330	17.165	0.1916	11	1.5010	14.0	(4 4 4)	61.751	30.876	0.3331
5	2.3900	40.0	(3 3 1)	37.603	18.802	0.2092	12	1.4570	6.0	(5 5 1)	63.832	31.916	0.3432
6	2.0060	20.0	(5 1 1)	45.162	22.581	0.2493	13	1.3560	8.0	(7 3 1)	69.229	34.615	0.3687
7	1.8400	55.0	(4 4 0)	49.496	24.748	0.2717							

PDF#35-1482: QM=Star(S); d=D:iffractometer; I=Diffraction											PDF Card		
Lead Oxide											(cSCR)		
Pb O													
Radiation=CuKα1				Lambda=1.54056				Filter=Ni					
Calibration=				2θ=17.762-86.924				I/Ic(RIR)=					
Ref: Boher, P. Private Communication (1984)													
Orthorhombic - (Unknown), Cmma (67)							Z=4 mp=						
CELL: 5.6085 x 5.6036 x 4.9893 <90.0 x 90.0 x 90.0>							P.S.=oC8 (\$GA) (O Pb)						
Density(c)=9.455		Density(m)=10.02A		Mwt=223.20		Vol=156.80		F(30)=965.8(0010,30/0)					
Ref: Boher, P., Garnier. C. R. Seances Acad. Sci., Ser. 2, v298 p203 (1984)													
NOTE: Preparation by thermal decomposition of lead dioxide \$GB-Pb O2 (Merck) at 793 K. Low temperature phase-transition. \$GA-PbO = \$GA-PbO orthorhombic at 200 K. See ICSD 62846, 62847, 62848, 62849 (PDF 78-1663, 64, 65, 78-1666).													
Color: Violet-red													
Strong Lines: 3.10/X 2.80/2 1.98/2 1.67/2 1.86/1 2.49/1 1.55/1 1.53/1 1.28/1 1.21/1													
42 Lines, Wavelength to Compute Theta = 1.54056Å(Cu), I%-Type = (Unknown)													
#	d(Å)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	#	d(Å)	I(f)	(h k l)	2-Theta	Theta	1/(2d)
1	4.9893	3.0	(0 0 1)	17.762	8.881	0.1002	22	1.4021	2.0	(4 0 0)	66.648	33.324	0.3566
2	3.1037	100.0	(1 1 1)	28.740	14.370	0.1611	23	1.4009	2.0	(0 4 0)	66.713	33.356	0.3569
3	2.8042	16.0	(2 0 0)	31.887	15.943	0.1783	24	1.3498	0.0	(4 0 1)	69.593	34.796	0.3704
4	2.8018	16.0	(0 2 0)	31.915	15.957	0.1785	25	1.3487	0.0	(0 4 1)	69.658	34.829	0.3707
5	2.4946	11.0	(0 0 2)	35.971	17.986	0.2004	26	1.2773	6.0	(3 3 1)	74.178	37.089	0.3915
6	2.4446	0.0	(2 0 1)	36.733	18.367	0.2045	27	1.2740	0.0	(2 2 3)	74.402	37.201	0.3925
7	2.4430	0.0	(0 2 1)	36.758	18.379	0.2047	28	1.2539	3.0	(4 2 0)	75.803	37.902	0.3988
8	2.1113	1.0	(1 1 2)	42.795	21.398	0.2368	29	1.2532	3.0	(2 4 0)	75.853	37.927	0.3990
9	1.9820	16.0	(2 2 0)	45.740	22.870	0.2523	30	1.2473	1.0	(0 0 4)	76.276	38.138	0.4009
10	1.8639	13.0	(2 0 2)	48.820	24.410	0.2683	31	1.2223	2.0	(4 0 2)	78.128	39.064	0.4091
11	1.8632	13.0	(0 2 2)	48.839	24.420	0.2684	32	1.2215	2.0	(0 4 2)	78.189	39.095	0.4093
12	1.8420	0.0	(2 2 1)	49.439	24.719	0.2714	33	1.2160	0.0	(4 2 1)	78.611	39.305	0.4112
13	1.6710	16.0	(3 1 1)	54.899	27.450	0.2992	34	1.2155	0.0	(2 4 1)	78.649	39.325	0.4114
14	1.6699	16.0	(1 3 1)	54.939	27.469	0.2994	35	1.2131	5.0	(3 1 3)	78.835	39.418	0.4122
15	1.6631	0.0	(0 0 3)	55.182	27.591	0.3006	36	1.2127	5.0	(1 3 3)	78.866	39.433	0.4123
16	1.5518	11.0	(2 2 2)	59.521	29.761	0.3222	37	1.1898	0.0	(1 1 4)	80.692	40.346	0.4202
17	1.5336	11.0	(1 1 3)	60.300	30.150	0.3260	38	1.1677	0.0	(3 3 2)	82.547	41.274	0.4282
18	1.4454	0.0	(3 1 2)	64.406	32.203	0.3459	39	1.1397	2.0	(2 0 4)	85.042	42.521	0.4387
19	1.4447	0.0	(1 3 2)	64.441	32.220	0.3461	40	1.1395	2.0	(0 2 4)	85.061	42.530	0.4388
20	1.4304	0.0	(2 0 3)	65.164	32.582	0.3496	41	1.1203	4.0	(4 2 2)	86.875	43.438	0.4463
21	1.4301	0.0	(0 2 3)	65.179	32.590	0.3496	42	1.1198	4.0	(2 4 2)	86.924	43.462	0.4465

PDF#36-1462: QM=Star(S); d=Diffraction; I=Diffraction											PDF Card		
Lead Nitrate											(cSCR)		
Pb (NO ₃) ₂													
Radiation=CuKα1			Lambda=1.5405981			Filter=Graph							
Calibration=Internal(Si)			2θ=19.564-127.853			I/c(RIR)=							
Ref: McMurdie, H., Morris, M., Evans, E., Paretzkin, B., Wong-Ng, W., Ettlinger, L., Hubbard, C.													
Powder Diffraction, v1 p70 (1986)											CAS#: 10099-74-8		
Cubic - Powder Diffraction, Pa-3 (205)						Z=4		mp=					
CELL: 7.8594 x 7.8594 x 7.8594 <90.0 x 90.0 x 90.0>											P.S=cP36 (?)		
Density(c)=4.532		Density(m)=5.02A		Mwt=331.21		Vol=485.48		F(30)=79.9(.0092,41/0)					
Ref: 1. Vegard, L.													
Z. Phys., v9 p395 (1922)													
NOTE: The sample was obtained from the J.T. Baker Chemical Company, Phillipsburg, New Jersey, USA. The structure was determined by Vegard (1). The mean temperature of data collection was 25.4 C. To replace 6-151 (2). References to other early patterns and structures will be found in reference (2).													
Color: Colorless													
Strong Lines: 4.53/X 2.37/8 2.27/5 3.93/4 2.78/4 1.80/3 1.76/2 1.60/2 1.51/2 1.97/2													
42 Lines, Wavelength to Compute Theta = 1.54056Å(Cu), I%-Type = Peak Height													
#	d(Å)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	#	d(Å)	I(f)	(h k l)	2-Theta	Theta	1/(2d)
1	4.5338	100.0	(1 1 1)	19.564	9.782	0.1103	22	1.3480	0.0	(4 3 3)	69.696	34.849	0.3709
2	3.9281	39.0	(2 0 0)	22.617	11.309	0.1273	23	1.3283	17.0	(5 3 1)	70.886	35.443	0.3764
3	3.5132	8.0	(2 1 0)	25.330	12.665	0.1423	24	1.3098	10.0	(6 0 0)	72.046	36.023	0.3817
4	3.2081	5.0	(2 1 1)	27.785	13.893	0.1559	25	1.2750	0.0	(6 1 1)	74.338	37.169	0.3922
5	2.7771	38.0	(2 2 0)	32.206	16.103	0.1800	26	1.2427	5.0	(6 2 0)	76.608	38.304	0.4023
6	2.6182	0.0	(2 2 1)	34.219	17.110	0.1910	27	1.1985	7.0	(5 3 3)	79.987	39.994	0.4172
7	2.3694	77.0	(3 1 1)	37.942	18.971	0.2110	28	1.1849	6.0	(6 2 2)	81.098	40.549	0.4220
8	2.2686	51.0	(2 2 2)	39.697	19.848	0.2204	29	1.1346	1.0	(4 4 4)	85.512	42.756	0.4407
9	2.0990	0.0	(3 2 1)	43.059	21.529	0.2382	30	1.1005	6.0	(5 5 1)	88.844	44.422	0.4543
10	1.9650	17.0	(4 0 0)	46.158	23.079	0.2545	31	1.0899	4.0	(6 4 0)	89.943	44.972	0.4588
11	1.9062	0.0	(4 1 0)	47.669	23.834	0.2623	32	1.0503	8.0	(6 4 2)	94.343	47.171	0.4761
12	1.8522	1.0	(4 1 1)	49.150	24.575	0.2700	33	1.0233	8.0	(7 3 1)	97.661	48.830	0.4886
13	1.8030	27.0	(3 3 1)	50.583	25.291	0.2773	34	0.9824	1.0	(8 0 0)	103.272	51.636	0.5090
14	1.7572	23.0	(4 2 0)	51.997	25.998	0.2845	35	0.9603	2.0	(7 3 3)	106.666	53.333	0.5207
15	1.7149	0.0	(4 2 1)	53.380	26.690	0.2916	36	0.9530	6.0	(8 2 0)	107.854	53.927	0.5247
16	1.6753	0.0	(3 3 2)	54.748	27.374	0.2985	37	0.9263	4.0	(6 6 0)	112.526	56.263	0.5398
17	1.6042	18.0	(4 2 2)	57.394	28.697	0.3117	38	0.9075	6.0	(7 5 1)	116.151	58.076	0.5509
18	1.5418	1.0	(4 3 1)	59.949	29.974	0.3243	39	0.9016	4.0	(6 6 2)	117.379	58.690	0.5546
19	1.5123	18.0	(5 1 1)	61.239	30.620	0.3306	40	0.8786	3.0	(8 4 0)	122.491	61.245	0.5691
20	1.4591	0.0	(2 5 0)	63.727	31.864	0.3427	41	0.8627	4.0	(9 1 1)	126.467	63.234	0.5796
21	1.3894	8.0	(4 4 0)	67.339	33.670	0.3599	42	0.8576	6.0	(8 4 2)	127.853	63.927	0.5831

PDF#36-1474: QM=Star(S); d=Diffraction; I=Diffraction											PDF Card		
Nitratine											(Calcite)		
Na N O3													
Radiation=CuKa1				Lambda=1.5405981				Filter=Graph					
Calibration=Internal(Si)				2T=22.820-99.067				I/Ic(RIR)=					
Ref: McMurdie, H., Morris, M., Evans, E., Paretzkin, B., Wong-Ng, W., Hubbard, C.													
Powder Diffraction, v1 p97 (1986)											CAS#:7631-99-4		
Rhombohedral - Powder Diffraction, R-3c (167)											Z=6		
CELL: 5.0711 x 5.0711 x 16.8236 <90.0 x 90.0 x 120.0>											mp=		
Density(c)=2.260			Density(m)=2.41A			Mwt=84.99			Vol=374.67			F(30)=73.2(0102,400)	
Ref: (1) Bragg, W.													
Proc. R. Soc. London, v89 p468 (1914)													
NOTE: The sample was recrystallized from aqueous solution. The structure of Na N O3 was determined by Bragg (1) and confirmed by Wyckoff (2). Na N O3 exhibits rotational disorder above ~200 C. The average temperature of data collection was ~25 C. To replace 7-271. Optical data on synthetic material. To replace 7-271. See ICSD 16709 (PDF 72-1213); See ICSD 28828 (PDF 85-850); See ICSD 37091 (PDF 76-2243); See ICSD 2865 (PDF 70-1518); See ICSD 15332 (PDF 72-25).													
Color: Colorless													
Strong Lines: 3.04/X 2.31/3 1.90/2 2.81/1 2.13/1 2.54/1 1.88/1 1.65/1 3.89/1 1.63/1													
32 Lines, Wavelength to Compute Theta = 1.54056A(Cu), I%-Type = Peak Height													
#	d(A)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	#	d(A)	I(f)	(h k l)	2-Theta	Theta	1/(2d)
1	3.8936	4.0	(0 1 2)	22.820	11.410	0.1284	17	1.4022	2.0	(0 0 12)	66.644	33.322	0.3566
2	3.0378	100.0	(1 0 4)	29.377	14.689	0.1646	18	1.3656	1.0	(2 1 7)	68.675	34.338	0.3661
3	2.8060	14.0	(0 0 6)	31.866	15.933	0.1782	19	1.3352	0.0	(0 2 10)	70.468	35.234	0.3745
4	2.5365	8.0	(1 1 0)	35.357	17.679	0.1971	20	1.3028	1.0	(1 2 8)	72.489	36.244	0.3838
5	2.3116	26.0	(1 1 3)	38.929	19.464	0.2163	21	1.2675	1.0	(2 2 0)	74.852	37.426	0.3945
6	2.1253	9.0	(2 0 2)	42.499	21.249	0.2353	22	1.2271	1.0	(1 1 12)	77.768	38.884	0.4075
7	1.9464	3.0	(0 2 4)	46.626	23.313	0.2569	23	1.1816	0.0	(2 1 10)	81.370	40.685	0.4232
8	1.8972	17.0	(0 1 8)	47.910	23.955	0.2636	24	1.1699	1.0	(1 3 4)	82.361	41.180	0.4274
9	1.8809	8.0	(1 1 6)	48.350	24.175	0.2658	25	1.1554	1.0	(2 2 6)	83.625	41.813	0.4328
10	1.6522	5.0	(2 1 1)	55.580	27.790	0.3026	26	1.1247	1.0	(1 2 11)	86.453	43.226	0.4446
11	1.6284	4.0	(1 2 2)	56.463	28.232	0.3071	27	1.0889	1.0	(0 4 2)	90.047	45.024	0.4592
12	1.5439	1.0	(2 1 4)	59.857	29.929	0.3239	28	1.0623	1.0	(4 0 4)	92.960	46.480	0.4707
13	1.5185	0.0	(2 0 8)	60.963	30.482	0.3293	29	1.0541	0.0	(2 0 14)	93.895	46.947	0.4743
14	1.5050	2.0	(1 1 9)	61.571	30.786	0.3322	30	1.0257	0.0	(1 1 15)	97.356	48.678	0.4875
15	1.4887	2.0	(1 2 5)	62.320	31.160	0.3359	31	1.0225	0.0	(1 0 16)	97.753	48.876	0.4890
16	1.4639	3.0	(3 0 0)	63.498	31.749	0.3416	32	1.0125	0.0	(3 0 12)	99.067	49.533	0.4938

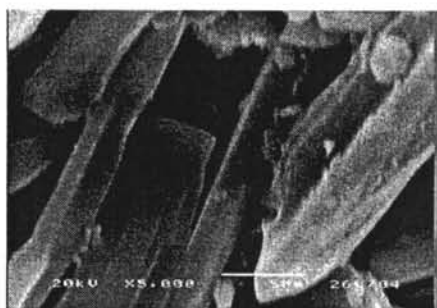
PDF#38-1477: QM=Star(S); d=Diffraction; I=Diffraction												PDF Card	
Massicot												(cSCR)	
Pb O													
Radiation=CuK α 1				Lambda=1.5405981				Filter=Graph					
Calibration=Internal(Ag FP)				2 θ =15.017-90.701				I/c(RIR)=					
Ref: McMurdie, H., Morris, M., Evans, E., Paretzkin, B., Wong-Ng, W., Zhang, Y. Powder Diffraction, v2 p46 (1987)												CAS#:1317-36-8	
Orthorhombic - Powder Diffraction, Pcam (57)								Z=4		mp=			
CELL: 5.4903 x 5.892 x 4.752 <90.0 x 90.0 x 90.0>								P.S.=oP8 (O Pb)					
Density(c)=9.644		Density(m)=10.02A		Mwt=223.20		Vol=153.72		F(30)=87.5(0062,55/0)					
Ref: (1) Leciejewicz, J. Acta Crystallogr., v14 p66 (1961)													
NOTE: The sample was obtained from Fisher Scientific Co., Fair Lawn, New Jersey, USA. The pattern is complicated by the presence of a small percentage of the red (tetragonal) form. Five weak reflections of the red form appear at d=3.1130, 2.8097, 2.5091, 1.8728 and 1.6780. The crystal structure of the yellow PbO was determined by Leciejewicz (1) and Kay (2) by means of neutron diffraction. The orthorhombic phase of PbO is stable above 500 C, the red form (litharge, tetragonal) is stable below 500 C (3). The mean temperature of data collection was 25.2 C. To replace 5-570 (4) and validated by calculated pattern. References to other early patterns will be found in Swanson and Fuyat (4). See ICSD 36250 (PDF 76-1796); See ICSD 15402 (PDF 72-93); See ICSD 15403 (PDF 72-94); See ICSD 60135 (PDF 77-1971).													
Color: Orange-yellow													
Strong Lines: 3.07/1 2.95/2 2.75/2 2.38/2 1.72/2 1.64/2 2.01/1 1.80/1 1.85/1 1.47/1													
37 Lines, Wavelength to Compute Theta = 1.54056A(Cu), I%-Type = Peak Height													
#	d(A)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	#	d(A)	I(f)	(h k l)	2-Theta	Theta	1/(2d)
1	5.8948	4.0	(0 1 0)	15.017	7.508	0.0848	20	1.4730	12.0	(0 4 0)	63.060	31.530	0.3395
2	4.0170	1.0	(1 1 0)	22.110	11.055	0.1245	21	1.4077	1.0	(3 1 2)	66.350	33.175	0.3552
3	3.0683	100.0	(1 1 1)	29.078	14.539	0.1630	22	1.3726	1.0	(4 0 0)	68.278	34.139	0.3643
4	2.9459	24.0	(0 2 0)	30.315	15.158	0.1697	23	1.3628	1.0	(1 4 1)	68.838	34.419	0.3669
5	2.7450	23.0	(2 0 0)	32.593	16.297	0.1821	24	1.3522	0.0	(1 2 3)	69.454	34.727	0.3698
6	2.4883	0.0	(2 1 0)	36.066	18.033	0.2009	25	1.3256	1.0	(2 3 2)	71.055	35.527	0.3772
7	2.3767	17.0	(2 0 1)	37.821	18.911	0.2104	26	1.2981	2.0	(2 4 0)	72.795	36.397	0.3852
8	2.2787	1.0	(1 2 1)	39.514	19.757	0.2194	27	1.2887	3.0	(3 3 1)	73.412	36.706	0.3880
9	2.2032	0.0	(0 1 2)	40.928	20.464	0.2269	28	1.2520	2.0	(0 4 2)	75.942	37.971	0.3994
10	2.0078	13.0	(2 2 0)	45.119	22.559	0.2490	29	1.2444	2.0	(4 2 0)	76.487	38.243	0.4018
11	1.9657	2.0	(0 3 0)	46.191	23.095	0.2546	30	1.2032	4.0	(1 3 3)	79.615	39.807	0.4156
12	1.8494	12.0	(0 2 2)	49.229	24.614	0.2704	31	1.1882	2.0	(0 0 4)	80.822	40.411	0.4208
13	1.7964	13.0	(2 0 2)	50.782	25.391	0.2783	32	1.1737	3.0	(3 1 3)	82.031	41.015	0.4260
14	1.7477	0.0	(3 1 0)	52.304	26.152	0.2861	33	1.1392	2.0	(1 1 4)	85.087	42.544	0.4389
15	1.7232	16.0	(1 3 1)	53.103	26.552	0.2902	34	1.1198	2.0	(1 5 1)	86.929	43.464	0.4465
16	1.6401	15.0	(3 1 1)	56.023	28.012	0.3049	35	1.1020	3.0	(4 2 2)	88.690	44.345	0.4537
17	1.5979	0.0	(2 3 0)	57.639	28.820	0.3129	36	1.0902	1.0	(2 0 4)	89.907	44.953	0.4586
18	1.5336	11.0	(2 2 2)	60.299	30.150	0.3260	37	1.0827	1.0	(2 5 0)	90.701	45.350	0.4618
19	1.5138	0.0	(0 3 2)	61.172	30.586	0.3303							

PDF#40-0099: QM=Star(S); d=(Unknown); f=(Unknown)													PDF Card
Lead Titanium Oxide													
Pb Ti O3													
Radiation=CuKa				Lambda=1.5418				Filter=Ni					
Calibration=				2T=22.433-56.935				I/c(RIR)=					
Ref: Yamaguchi, O., Narai, A., Komatsu, T., Shimizu, K. J. Am. Ceram. Soc., v69 pC256 (1986)													
Cubic - (Unknown), Z= mp=													
CELL: 3.961 x 3.961 x 3.961 <90.0 x 90.0 x 90.0> P.S=c70 (Perovskite, Ca O3 Ti)													
Density(c)=8.099				Density(m)=7.57A		Mwt=303.10		Vol=62.15		F(6)=79.0(0127,6/0)			
Ref: Ibid.													
NOTE: C phase. Made using Pb (O C3 H7)2 and Ti (O C3 H7)4. Reflections somewhat broad. Pattern taken at 680 C.													
Strong Lines: 2.80/X 2.29/4 3.96/4 1.98/4 1.62/4 1.77/1 0.00/1 0.00/1 0.00/1 0.00/1													
6 Lines, Wavelength to Compute Theta = 1.54056A(Cu), P%-Type = (Unknown)													
#	d(A)	I(f)	(h k l)	2-Theta	Theta	1/(2d)	#	d(A)	I(f)	(h k l)	2-Theta	Theta	1/(2d)
1	3.9600	35.0	(1 0 0)	22.433	11.216	0.1263	4	1.9800	35.0	(2 0 0)	45.788	22.894	0.2525
2	2.8010	100.0	(1 1 0)	31.924	15.962	0.1785	5	1.7710	10.0	(2 1 0)	51.563	25.782	0.2823
3	2.2870	40.0	(1 1 1)	39.365	19.683	0.2186	6	1.6160	35.0	(2 1 1)	56.935	28.467	0.3094

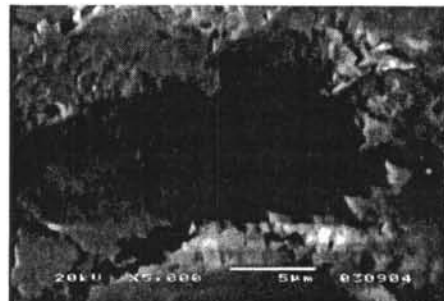
PDF#50-0346: QM=Star(S); d=Diffraction; I=Diffraction													PDF Card	
Lead Titanium Zirconium Oxide													(fFERRIC)	
Pb (Zr0.44 Ti0.56) O3														
Radiation=CuKa1			Lambda=1.54056			Filter=								
Calibration=			2 θ =21.442-155.720			I/Ic(RIR)=								
Ref. Jin, Z., Testing & Analysis Centre, Suzhou Univ., P.R.China.														
ICDD Grant-in-Aid (1998)														
Tetragonal - (Unknown), P4mm (99)						Z=1		mp=						
CELL: 4.0172 x 4.0172 x 4.1391 <90.0 x 90.0 x 90.0>													P.S=IP5 (?)	
Density(c)=8.000		Density(m)=7.64A		Mwt=322.16		Vol=66.80		F(30)=92.3(,0108,30/0)						
Ref. Ibid.														
Color: Black														
Strong Lines: 2.88/X 2.84/4 2.34/2 1.65/2 4.02/2 2.01/2 4.14/2 1.67/1 2.07/1 1.44/1														
58 Lines, Wavelength to Compute Theta = 1.54056Å(Cu), I%-Type = Peak Height														
#	d(Å)	I(f)	(hkl)	2-Theta	Theta	1/(2 θ)	#	d(Å)	I(f)	(hkl)	2-Theta	Theta	1/(2 θ)	
1	4.1406	16.0	(0 0 1)	21.442	10.721	0.1208	30	1.0760	3.0	(3 2 1)	91.430	45.715	0.4647	
2	4.0195	18.0	(1 0 0)	22.097	11.048	0.1244	31	1.0347	0.0	(0 0 4)	96.223	48.112	0.4832	
3	2.8829	100.0	(1 0 1)	30.994	15.497	0.1734	32	1.0043	1.0	(4 0 0)	100.167	50.084	0.4979	
4	2.8424	37.0	(1 1 0)	31.447	15.724	0.1759	33	1.0022	1.0	(1 0 4)	100.455	50.227	0.4989	
5	2.3424	24.0	(1 1 1)	38.397	19.199	0.2135	34	0.9898	0.0	(2 2 3)	102.195	51.098	0.5052	
6	2.0689	10.0	(0 0 2)	43.717	21.858	0.2417	35	0.9722	1.0	(1 1 4)	104.803	52.402	0.5143	
7	2.0090	18.0	(2 0 0)	45.091	22.545	0.2489	36	0.9611	1.0	(3 0 3)	106.539	53.269	0.5202	
8	1.8398	5.0	(1 0 2)	49.502	24.751	0.2718	37	0.9483	1.0	(4 1 1)	108.638	54.319	0.5273	
9	1.8065	4.0	(2 0 1)	50.478	25.239	0.2768	38	0.9470	1.0	(3 3 0)	108.857	54.428	0.5280	
10	1.7972	3.0	(2 1 0)	50.757	25.379	0.2782	39	0.9346	0.0	(3 1 3)	111.011	55.506	0.5350	
11	1.6724	13.0	(1 1 2)	54.850	27.425	0.2990	40	0.9231	0.0	(3 3 1)	113.117	56.559	0.5417	
12	1.6480	21.0	(2 1 1)	55.732	27.866	0.3034	41	0.9198	1.0	(2 0 4)	113.742	56.871	0.5436	
13	1.4413	7.0	(2 0 2)	64.611	32.306	0.3469	42	0.9035	1.0	(4 0 2)	116.980	58.490	0.5534	
14	1.4206	3.0	(2 2 0)	65.670	32.835	0.3520	43	0.8982	2.0	(4 2 0)	118.092	59.046	0.5567	
15	1.3794	1.0	(0 0 3)	67.893	33.946	0.3625	44	0.8968	1.0	(2 1 4)	118.391	59.196	0.5575	
16	1.3569	2.0	(2 1 2)	69.177	34.588	0.3685	45	0.8816	0.0	(4 1 2)	121.790	60.895	0.5672	
17	1.3431	1.0	(2 2 1)	69.991	34.995	0.3723	46	0.8669	1.0	(3 2 3)	125.382	62.691	0.5768	
18	1.3390	0.0	(3 0 0)	70.236	35.118	0.3734	47	0.8610	1.0	(3 3 2)	126.923	63.461	0.5807	
19	1.3047	4.0	(1 0 3)	72.369	36.185	0.3832	48	0.8364	1.0	(2 2 4)	134.130	67.065	0.5978	
20	1.2740	4.0	(3 0 1)	74.402	37.201	0.3925	49	0.8240	1.0	(4 2 2)	138.394	69.197	0.6068	
21	1.2705	4.0	(3 1 0)	74.642	37.321	0.3935	50	0.8188	0.0	(3 0 4)	140.353	70.177	0.6106	
22	1.2412	1.0	(1 1 3)	76.719	38.359	0.4028	51	0.8120	0.0	(4 0 3)	143.107	71.554	0.6158	
23	1.2144	1.0	(3 1 1)	78.734	39.367	0.4117	52	0.8108	0.0	(1 0 5)	143.619	71.810	0.6167	
24	1.1712	2.0	(2 2 2)	82.247	41.124	0.4269	53	0.8034	1.0	(4 3 0)	146.982	73.491	0.6224	
25	1.1375	1.0	(2 0 3)	85.246	42.623	0.4396	54	0.8023	1.0	(3 1 4)	147.516	73.758	0.6232	
26	1.1242	1.0	(3 0 2)	86.500	43.250	0.4448	55	0.7950	1.0	(4 1 3)	150.846	75.423	0.6282	
27	1.1141	0.0	(3 2 0)	87.481	43.740	0.4488	56	0.7948	1.0	(1 1 5)	151.462	75.731	0.6291	
28	1.0945	3.0	(2 1 3)	89.461	44.731	0.4568	57	0.7887	1.0	(5 0 1)	155.185	77.593	0.6340	
29	1.0826	3.0	(3 1 2)	90.716	45.358	0.4619	58	0.7879	1.0	(5 1 0)	155.720	77.860	0.6346	

PDF#50-1430: QM=(Unknown); d=Calculated; I=Calculated											PDF Card		
Lead Oxide											(rSEM)		
Pb O2													
Radiation=MoKa				Lambda=0.71073				Filter=Zr					
Calibration=				2 θ =29.267-81.419				I/c(RIR)=					
Ref: Haines, J., C.N.R.S., Laboratoire de Physico-Chimie des Matériaux, Meudon, France. Private Communication (1998)													
Cubic - (Unknown), Pa-3 (205)						Z=4		mp=					
CELL: 5.2804 x 5.2804 x 5.2804 <90.0 x 90.0 x 90.0>													
Density(c)=10.791		Density(m)=9.24A		Mwt=239.20		Vol=147.23		F(B)=126.5(.0042,15/0)					
Ref: Haines, J., Leger, J.M., Schulte, O. Science, v271 p629 (1996)													
NOTE: Data obtained in situ at 9.0 GPa in a diamond-anvil cell. Transforms to orthorhombic phase at low pressure. See also 22-389 taken at 50 kbar. Intensities recorded with an image plate. Rietveld refinement.													
Strong Lines: 3.05/X 2.64/4 1.59/3 1.87/3 1.52/1 1.21/1 1.18/1 1.32/1 0.00/1 0.00/1													
8 Lines, Wavelength to Compute Theta = 1.54056Å(Cu), I%-Type = (Unknown)													
#	d(Å)	I(I)	(hkl)	2-Theta	Theta	1/(2d)	#	d(Å)	I(I)	(hkl)	2-Theta	Theta	1/(2d)
1	3.0490	100.0	(1 1 1)	29.267	14.633	0.1640	5	1.5240	10.0	(2 2 2)	60.720	30.360	0.3281
2	2.6400	40.0	(2 0 0)	33.928	16.964	0.1894	6	1.3200	3.0	(4 0 0)	71.401	35.700	0.3788
3	1.8670	32.0	(2 2 0)	48.734	24.367	0.2678	7	1.2110	9.0	(3 3 1)	78.999	39.499	0.4129
4	1.5920	33.0	(3 1 1)	57.874	28.937	0.3141	8	1.1810	8.0	(4 2 0)	81.410	40.710	0.4234

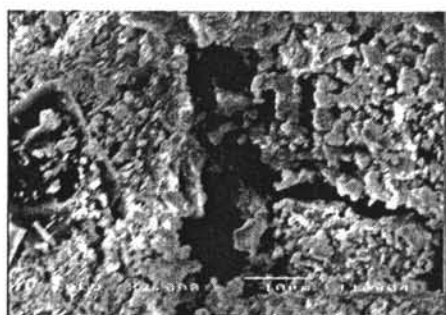
Appendix C The SEM microstructure of dried lead zirconate gels calcined at 200°, 300°, 400°, 500°, 600° and 700°C for 1 h at high magnification of 5000.



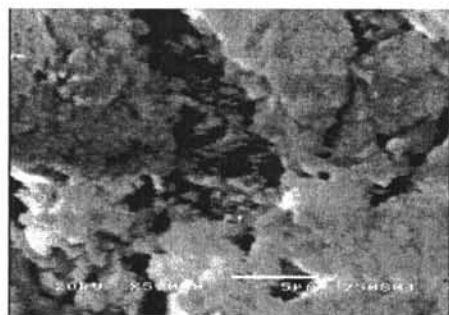
Dried PbZrO₃ gel



PbZrO₃ calcined at 500°C



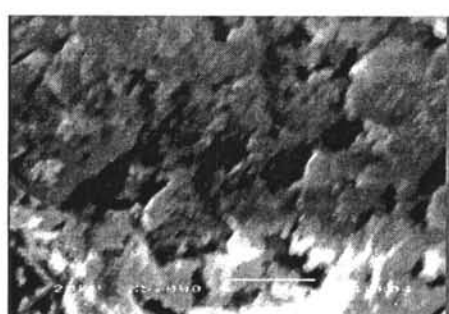
PbZrO₃ calcined at 200°C



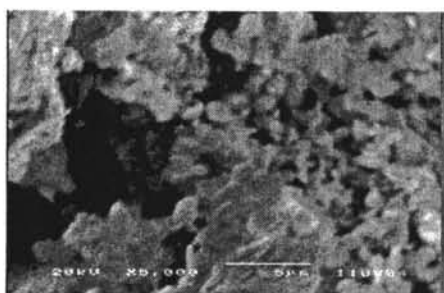
PbZrO₃ calcined at 600°C



PbZrO₃ calcined at 300°C

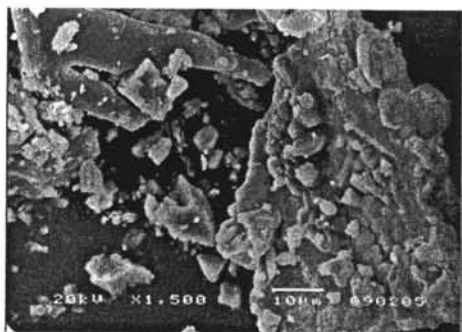


PbZrO₃ calcined at 700°C

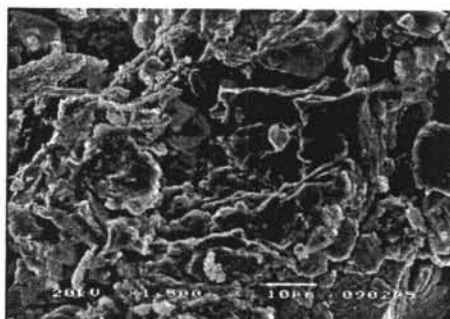


PbZrO₃ calcined at 400°C

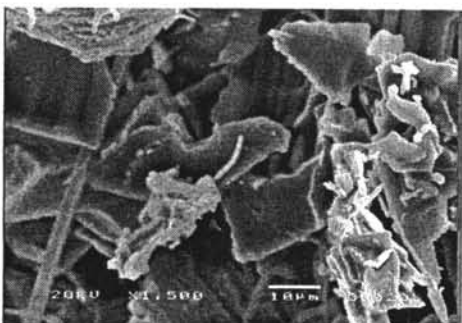
Appendix D The SEM microstructure of dried lead zirconate titanate gels of PZT 1 ; PZT 2 ; PZT 3 ; PZT 4 ; PZT 5; PZT 6; PZT 7 at same magnification of 1500.



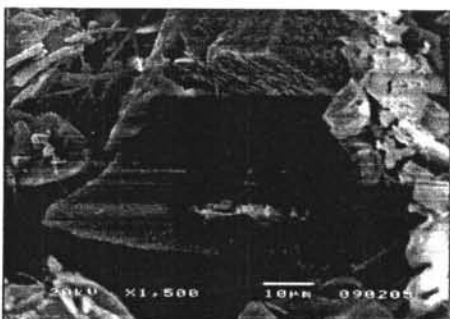
PZT 1



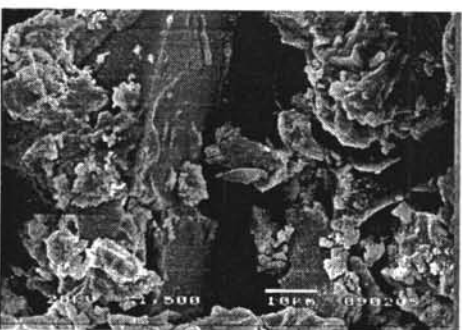
PZT 5



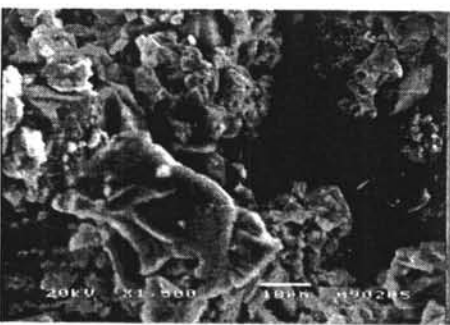
PZT 2



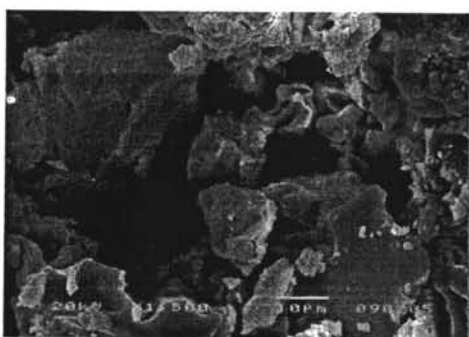
PZT 6



PZT 3



PZT 7



PZT 4

Appendix E The electrical property preparation and calculation.

The samples were prepared according to the ASTM B263-94 standard for electrical property measurements. Pellet samples were prepared as a thin disc having 12 mm in diameter and 0.50 mm in thickness. In our experiment, the electrical properties, the dielectric constant, tan delta and electrical conductivity were measured in the frequency range between 10^3 - 10^6 Hz and at room temperature.

Macroscopic description: Ohm's law

$$V = IR \quad (\text{eq1})$$

voltage drop across medium [V] = [J/C]

I : current through medium [A] = [C/s]

R: resistance of medium [Ω] = [J.s/C²]

Eliminating extensive variables by substitutions:

$$R = d/A\sigma = d\rho/A$$

$$\sigma = 1/\rho$$

d : thickness of medium [m]

A : cross-sectional area of medium [m²]

σ : electrical conductivity of medium [1/ Ω .m] = [C²/J.s.m]

ρ : resistivity of medium; = σ^{-1}

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2. Tangboriboon, N., Jamieson, A.M., Sirivat, A., and Wongkasemjit, S. (2006) A Novel Route to Perovskite Lead Titanate from Lead and Titanium Glycolates via Sol-Gel Process. *Appl. Org. Chem.*, accepted (July 15, 2006).
3. Tangboriboon, N., Jamieson, A.M., Sirivat, A., and Wongkasemjit, S. (2006) A Novel Route to Perovskite Lead Zirconate from Lead Glycolate and Sodium tris(glycozirconate) via Sol-Gel Process. *Mater. Chem. Phys.*, submit.
4. Tangboriboon, N., Jamieson, A.M., Sirivat, A., and Wongkasemjit, S. (2006) A Novel Route to Perovskite Lead Zirconate Titanate (PZT) from Lead Glycolate, Sodium tris(glycozirconate), and Titanium glycolate via Sol-gel Process *Mac. Mol.*, submit.

Proceedings:

1. Tangboriboon, N., Jameison, A. M., Sirivat, A., and Wongkasemjit, S. (2006, May) A New Route to Electrical Perovskite Lead Titanate via Sol-Gel Process. Conference at Society for the Advancement of Material and Process Engineering (SAMPE '06), Long Beach Convention Center, Long Beach, California, USA.

Presentations:

1. Tangboriboon, N., Pakdeewanishsukho, K., Jamieson, A. M., Sirivat, A., and Wongkasemjit, S. (2006, February) Electrical Properties of a Novel Lead Alkoxide Precursor: Lead Glycolate. Paper presented at the 44th Kasetsart University Annual Conference, Bangkok, Thailand.
2. Tangboriboon, N., Jamieson, A.M., Sirivat, A., and Wongkasemjit, S. (2006, March) A Novel Route to Perovskite Lead Titanate from Lead and Titanium Glycolates via Sol-Gel Process. Paper presented at the 17th International Zurich Symposium on Electromagnetic Compatibility, The Suntec Singapore International Convention & Exhibition Centre, Singapore.