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Unit-cell data of the lead niobate $PbNb_2O_6$.

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The X-ray diffraction powder pattern of the ferroelectric form of a specimen of pure $PbNb_2O_6$, melted in a platinum crucible at 1350° C., can be indexed on the basis of an orthorhombic unit cell with $a = 17{\cdot}63$, $b = 17{\cdot}93$, $c = 3{\cdot}868$ Å. The powder pattern shows no sign of diffraction peaks caused by a cell with the c axis equal to twice that used, as was originally suggested by Goodman (1953) and Francombe (1956) on the basis of single-crystal data. The pattern, as indexed in Table 1, obeys the extinction rule hkl with $h+k = 2n$. This extinction rule fits only two possible space groups, D_2^6–$C222$ and C_{2v}^{11}–$Cmm2$, and the compound would then have 10 molecules to the unit cell.

Table 1. *X-ray powder diffraction data for high-temperature form of* $PbNb_2O_6$

(Cu $K\alpha_1$ radiation)

hkl	d_o (Å)	I_o	*hkl*	d_o (Å)	I_o
220	6·25	10	261	2·2838	5
130	5·63	50	800	2·2030	5
310	5·56	20	280	2·1726	20
040	4·476	10	820	2·1396	25
400	4·405	5	711	2·0961	5
240	3·988	10	660	2·0942	10
420	3·948	5	750	2·0615	5
001	3·859	5	371	2·0073	10
150	3·508	25	480	1·9976	15
510	3·453	20	190	1·9803	10
221	3·288	20	840	1·9766	10
131	3·187	95	002	1·9340	60
311	3·176	100	281	1·8952	10
440	3·138	15	390	1·8875	20
350	3·057	80	821	1·8725	5
530	3·033	85	930	1·8621	10
060	2·985	30	661	1·8433	20
600	2·934	35	312	1·8277	5
041	2·926	40	0,10,0	1·7944	5
401	2·902	25	680	1·7823	5
260	2·827	50	860	1·7755	10
620	2·788	35	10,0,0	1·7631	25
241	2·776	55	2,10,0	1·7590	20
421	2·763	85	242	1·7406	15
151	2·599	15	422	1·7360	10
511	2·577	20	950	1·7211	5
170	2·536	5	391	1·6972	5
441	2·4383	5	152	1·6949	5
351	2·4000	10	931	1·6786	5
061	2·3641	10	442	1·6480	5
370	2·3468	5	352	1·6361	20
730	2·3195	5	532	1·6321	30

High-temperature X-ray patterns were made on the same specimen in an attempt to determine the symmetry of pure $PbNb_2O_6$ above its reported Curie temperature of 570° C. At 700° C. it was found that this specimen had reverted almost completely to the low-temperature non-ferroelectric form described by Francombe (1956), and this form remained stable at room temperature. However, a specimen of $PbNb_2O_6$+2wt.% $ZrTiO_4$ was apparently completely stable in the 'high-temperature' form from room temperature to 700° C. This single phase solid solution at room temperature has a and b parameters very little different from the pure material but a c parameter of 3·873 Å. At 600° C. it was found that the close doublets formerly associated with orthorhombic symmetry were no longer present and the powder pattern could be completely indexed on the basis of a tetragonal unit cell with $a = 12{\cdot}56$, $c = 3{\cdot}925$ Å (Table 2). This pattern has only one extinction rule of $0kl$ with $k = 2n$. Three space groups are possible for this tetragonal symmetry, namely C_{4v}^2–$P4bm$, D_{2d}^7–$P\bar{4}b2$ and D_{4h}^5–$P4/mbm$. As the tetragonal structure is no longer ferroelectric it is probable that the material has a center of symmetry; if so, the space group would be D_{4h}^5–$P4/mbm$.

Table 2. *High-temperature X-ray diffraction data for* $PbNb_2O_6$+2 wt.% $ZrTiO_4$ *at* 600° C.

(Cu $K\alpha_1$ radiation)

d_o (Å)	I_o	$a = 12{\cdot}56$ Å *hkl*
6·26	5	020
5·61	45	120
4·436	5	220
3·928	5	001
3·482	30	320
3·326	15	021
3·215	100	121
3·140	15	040
3·046	100	140
2·955	60	330
2·945	70	221
2·806	65	240
2·793	100	131
2·605	35	231
2·4505	5	041
2·4049	5	141
2·3339	10	250
2·1562	20	350
2·0961	15	060
1·9868	60	260
1·9624	80	002
1·8908	10	351
1·8717	15	{022, 360}
1·8489	10	061
1·7787	10	170/550
1·7729	15	261
1·7609	25	132
1·7564	30	451
1·7113	10	232
1·6914	10	361
1·6504	60	142
1·6195	40	171/551
1·6101	50	242

References

Francombe, M. H. (1956). *Acta Cryst.* **9**, 683.
Goodman, G. (1953). *J. Amer. Ceram. Soc.* **36**, 368.