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Unit Cell and Space Group of $SrPbO_3$*

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$SrPbO_3$ is orthorhombic with $a = 5.8595 \pm 5$, $b = 5.9568 \pm 5$, and $c = 8.3253 \pm 6$ Å. The probable space group is *Pbnm*.

Weiss (*1*) and Hoppe and Blinne (*2*) first prepared $SrPbO_3$. Weiss stated that $SrPbO_3$ is probably an orthorhombic perovskite with space group *Pbnm* or $Pbn2_1$ (*1*). This finding is consistent with data on other $A^{2+}B^{4+}O_3$ orthorhombically distorted perovskites. Keester and White (*3*) have recently prepared polycrystalline $SrPbO_3$ and report diffractometer data which are presumably of higher precision than those of Weiss. They find similar cell dimensions but have chosen a different and incorrect space group because the resolution of their diffractometer was not sufficient to distinguish between *Pnma*: [(*Okl*) $k + l = 2n$ and (*hkO*) $h = 2n$] and *Pbnm*: [(*hOl*) $h + l = 2n$ and (*Okl*) $k = 2n$]. In this note, diffraction patterns taken on a Hägg–Guinier camera are used to show that the space group of $SrPbO_3$ should be *Pbnm*.

In a recent study, samples of single crystal and polycrystalline $BaPbO_3$ were prepared (*4*). $BaPbO_3$ was found to be an orthorhombically distorted perovskite with space group *Pbnm* or $Pbn2_1$ based on single crystal precession patterns and Guinier powder diffraction data. Space group *Pbnm* was assumed by analogy with other orthorhombic perovskites. Guinier data taken on $SrPbO_3$ prepared in a manner similar to that for $BaPbO_3$ did not indicate a unit cell and space group different from those of Weiss. Thus, we did not mention this work in our earlier publication. However, in light of Keester and White's results it seems worthwhile to report our data.

The sample was prepared by thoroughly mixing spectroscopic grade $SrCO_3$ and reagent grade PbO_2, pelletizing, and heating in a Pt foil envelope

TABLE I

POWDER DIFFRACTION DATA FOR $SrPbO_3$

$h\ k\ l$	d_{calcd}	d_{obsd}	I_{obsd}
1 1 0	4.1773	4.1835	90
0 0 2	4.1626	4.1635	90
1 1 1	3.7336	3.7336	30
0 2 0	2.9784	2.9788	95
1 1 2	2.9486	2.9453	100
2 0 0	2.9297	2.9312	100
0 2 1	2.8044	2.8047	15
2 1 0	2.6290	2.6287	5
1 2 1	2.5296	2.5297	5
1 0 3	2.5080	2.5073	25
2 1 1	2.5070		
0 2 2	2.4222	2.4221	50
2 0 2	2.3958	2.3957	50
1 1 3	2.3115	2.3117	20
1 2 2	2.2385	2.2382	10
2 2 0	2.0886	2.0880	95
0 0 4	2.0813	2.0818	95
0 2 3	2.0304	2.0303	20
2 2 1	2.0259	2.0258	25
2 1 3	1.9085	1.9088	5
1 3 0	1.8806	1.8805	70
2 2 2	1.8668	1.8665	85
1 1 4	1.8629	1.8633	85
3 1 0	1.8559	1.8560	50
1 3 1	1.8343	1.8344	35
3 1 1	1.8115	1.8117	10
1 3 2	1.7138	1.7136	95
0 2 4	1.7060	1.7061	90
2 0 4	1.6967	1.6970	95
3 1 2	1.6951	1.6942	95
2 2 3	1.6688	1.6688	5
1 3 3	1.5568	1.5569	15

*Contribution No. 1743.

TABLE I—*continued*

h k l	d_{calcd}	d_{obsd}	I_{obsd}
0 4 0	1.4892	1.4892	50
2 2 4	1.4743	1.4742	95
0 4 1	1.4660	1.4649	60
4 0 0	1.4649		
0 4 2	1.4022	1.4022	40
4 1 1	1.4022		
1 3 4	1.3953	1.3954	60
3 3 0	1.3924	1.3925	35
0 0 6	1.3875	1.3874	15
3 1 4	1.3852	1.3852	45
4 0 2	1.3818	1.3818	30
3 3 1	1.3733	1.3733	10
2 4 0	1.3275	1.3275	60
3 3 2	1.3205	1.3204	85
1 1 6	1.3168	1.3168	90
4 2 0	1.3145	1.3146	75
0 4 3	1.3122	1.3111	20
2 4 1	1.3110		
2 2 5	1.3020	1.3020	5

for 24 hr at 900°C. The product was reground, repelletized, and reheated under the same conditions. Table I shows an X-ray diffraction pattern taken on a Hägg–Guinier camera according to the procedure described earlier (*4*). The pattern has been slightly overexposed to bring out weak lines. The increased resolution characteristic of the Guinier patterns makes indexing considerably more reliable than in the diffractometer pattern of Keester and White. Although the space group is not unequivocally determined by this pattern, the indexing is consistent with the space group *Pbnm* or $Pbn2_1$ as indicated by Weiss. The cell dimensions obtained from least-squares analysis of the data in space group *Pbnm* are: $a = 5.8595 \pm 5$, $b = 5.9568 \pm 5$, and $c = 8.3253 \pm 6$ Å.

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