Modulated crystal structure of Pr_2SbO_2

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Supplementary Materials

Pr_2SbO_2
idealized structure

*I*4/*mmm* *I* 4/*m* 2/*m* 2/*m* (no. 139)

a = 13.7017 Å
b = *c* = 3.9957 Å

*t*2

Immm *I* 2/*m* 2/*m* 2/*m* (no. 71)

*t*2

Pmmm *P* 2/*m* 2/*m* 2/*m* (no. 47)

*i*2

a, 2***b***, ***c***

a = 13.7017 Å
b = 7.9914 Å
c = 3.9957 Å

Pmmm *P* 2/*m* 2/*m* 2/*m* (no. 47)

Pr_2SbO_2
Motif 1

Sb: 2*a*	Pr: 4*e*	O: 4*d*
4/*mmm*	4*mm*	$\bar{4}m2$
0	0.3362	¼
0	0	½
0	0	0

2*a*	4*i*	4*j*
mmm	*mm*2	*mm*2
0	0.3362	0.25
0	0	½
0	0	0

1*a*	1*h*	2*q*	2*t*	2*s*	2*r*
mmm	*mmm*	*mm*2	*mm*2	*mm*2	*mm*2
0	½	0.3362	0.3362	0.25	0.25
0	½	0	½	½	0
0	½	0	½	0	½

2*i*	2*j*	2*q*	2*s*	4*x*	4*w*	2*t*	2*r*
2*mm*	2*mm*	*mm*2	*mm*2	.*m*.	.*m*.	*mm*2	*mm*2
0	½	0.3362	0.3362	0.3362	0.25	0.25	0.25
0.18	0.18	0	½	0.25	0.25	½	0
0	0	0	0	½	0	½	½

Fig. 1. Group-subgroup relations between idealized Structure of Pr_2SbO_2 (which is identical to Pr_2BiO_2) and structure with ordered Sb-dumbbells (motif 1, Fig. 12b).

Pr_2SbO_2
idealized structure

$I4/mmm$ $I\,4/m\,2/m\,2/m$ (no. 139)

a = 13.7017 Å
$b = c$ = 3.9957 Å

$t2$

$P\bar{4}$ $P\,\bar{4}\,1\,1$ (no. 81)

$t2$

¼, ¼, ¼

$P4_2/n$ $P\,4_2/n\,1\,1$ (no. 86)
Origin choice 2

$i5$

$\boldsymbol{a}$-2$\boldsymbol{b}$, 2$\boldsymbol{a}$+$\boldsymbol{b}$, $\boldsymbol{c}$

$P4_2/n$ $P\,4_2/n\,1\,1$ (no. 86)
Origin choice 2

a = 13.7017 Å
$b = c$ = 8.9347 Å

$t2$

¼, ¼, ¼

$I4/m$ $I\,4/m\,1\,1$ (no. 87)

Pr_2SbO_2
Motif 3

Sb: 2*a* 4/*mmm*	Pr: 4*e* 4*mm*	O: 4*d* $\bar{4}m2$
0 0 0	0.3362 0 0	¼ ½ 0

2*a* 4/*m*	4*e* 4..	4*d* $\bar{4}$..
0 0 0	0.3362 0 0	¼ ½ 0

2*a* $\bar{4}$..	4*f* 2..	4*e* 2..
¾ ¾ ¾	0.0862 ¾ ¾	0.0 ¾ ¼

2*b* $\bar{4}$..	8*g* 1	8*g* 1	8*g* 1	4*f* 2..	8*g* 1	8*g* 1	4*e* 2..
¼ ¾ ¾	0.75 0.85 0.45	0.0862 0.85 0.45	0.0862 0.05 0.85	0.9138 ¾ ¾	0 0.15 0.05	0.5 0.35 0.45	0 ¾ ¼

1*a* $\bar{4}$..	4*h* 1	4*h* 1	4*h* 1	2*e* 2..	4*h* 1	4*h* 1	2*g* 2..
½ 0 0	0.0 0.07 0.645	0.8362 0.6 0.2	0.8362 0.8 0.6	0.1638 0 0	0.25 0.3 0.6	0.25 0.1 0.2	0.25 ½ 0
1*b* $\bar{4}$..	4*h* 1	4*h* 1	4*h* 1	2*f* 2..	4*h* 1	4*h* 1	2*g* 2..
0 ½ ½	0.5 0.57 0.145	0.3362 0.7 0.9	0.3362 0.1 0.7	0.6638 ½ ½	0.75 0.9 0.8	0.75 0.7 0.4	0.75 ½ 0

Fig. 2. Group-subgroup relations between idealized Structure of Pr_2SbO_2 (which is identical to Pr_2BiO_2) and structure with ordered Sb-dumbbells and isolate Sb-atoms (motif 3, Fig. 12d).

Pr_2SbO_2
idealized structure

*I*4/*mmm* *I* 4/*m* 2/*m* 2/*m* (no. 139)

a = 13.7017 Å
b = *c* = 3.9957 Å

Sb: 2*a*	Pr: 4*e*	O: 4*d*
4/*mmm*	4*mm*	$\bar{4}m2$
0	0.3362	¼
0	0	½
0	0	0

*t*2

Immm *I* 2/*m* 2/*m* 2/*m* (no. 71)

2*a*	4*i*	4*j*
mmm	*mm*2	*mm*2
0	0.3362	0.25
0	0	½
0	0	0

*t*2

Pmmm *P* 2/*m* 2/*m* 2/*m* (no. 47)

1*a*	1*h*	2*q*	2*t*	2*s*	2*r*
mmm	*mmm*	*mm*2	*mm*2	*mm*2	*mm*2
0	½	0.3362	0.3362	0.25	0.25
0	½	0	½	½	0
0	½	0	½	0	½

*t*2

P2/m *P* 1 2/*m* 1 (no. 10)

1*a*	1*h*	2*m*	2*n*	2*n*	2*m*
2/*m*	2/*m*	*m*	*m*	*m*	*m*
0	½	0.3362	0.3362	0.25	0.25
0	½	0	½	½	0
0	½	0	½	0	½

*t*2

$P\bar{1}$ $P\bar{1}$ (no. 2)

1*a*	1*h*	2*i*	2*i*	2*i*	2*i*
$\bar{1}$	$\bar{1}$	1	1	1	1
0	½	0.3362	0.3362	0.25	0.25
0	½	0	½	½	0
0	½	0	½	0	½

*t*2

1*a* 1	1*a* 1	1*a* 1	1*a* 1	1*a* 1	1*a* 1
0 0 0	½ ½ ½	0.3362 0 0	0.6623 0 0	0.25 ½ 0	0.75 ½ 0
		1*a* 1	1*a* 1	1*a* 1	1*a* 1
		0.3362 ½ ½	0.1623 ½ ½	0.25 0 ½	0.75 0 ½

*P*1 *P* 1 (no. 1)

*i*8

a, 4***b***, 2***c***

a = 13.7017 Å
b = 15.9828 Å
c = 7.9914 Å

*P*1 *P* 1 (no. 1)

Pr_2SbO_2
Motif 4

Fig. 3. Group-subgroup relations between idealized Structure of Pr_2SbO_2 (which is identical to Pr_2BiO_2) and structure with ordered Sb-dumbbells and isolate Sb-atoms (motif 4, Fig. 12e).