High Temperature $SmBaMn_2O_6$ Structure: AB2C6D_oC40_65_g_n_ijklm_h-001

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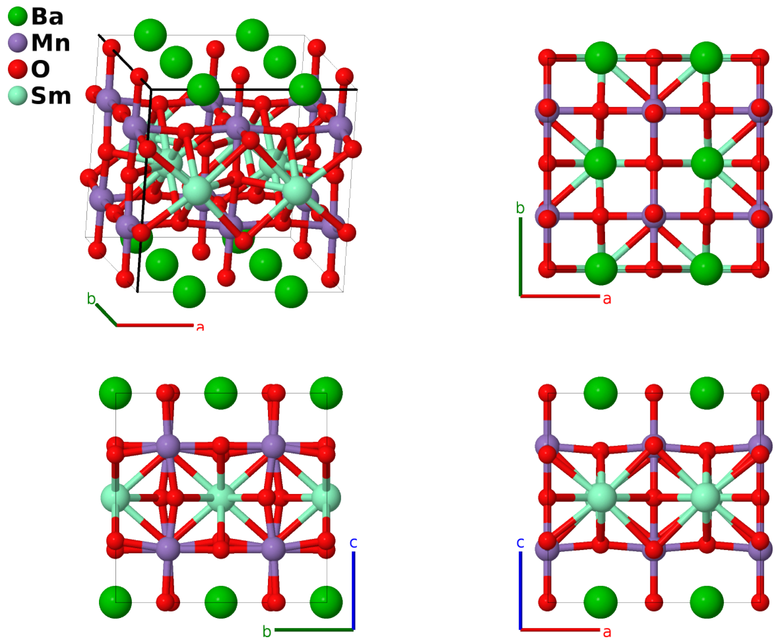
https://aflow.org/p/VMAN

https://aflow.org/p/AB2C6D_oC40_65_g_n_ijklm_h-001



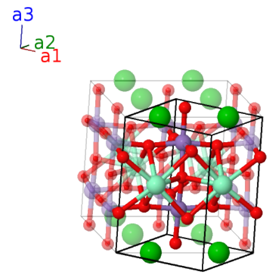
Prototype	$BaMn_2O_6Sm$
AFLOW prototype label	AB2C6D_oC40_65_g_n_ijklm_h-001
ICSD	none
Pearson symbol	oC40
Space group number	65
Space group symbol	*Cmmm*
AFLOW prototype command	`aflow --proto=AB2C6D_oC40_65_g_n_ijklm_h-001 --params=`$a, b/a, c/a, x_1, x_2, y_3, y_4, z_5, z_6, z_7, y_8, z_8$

- $SmBaMn_2O_6$ undergoes several structural and magnetic phase transitions with changing temperature (Sagayama, 2014; Chen, 2019):
  - Below 190K the structure is in a polar orthorhombic phase with space group $Pmc2_1$ #26.
  - Between 190K and 362 K the structure is in a non-polar orthorhombic phase with space group *Pnma* #62.
  - Above 362 K the structure is in quadrupled perovskite orthorhombic phase with space group *Cmmm* #65 (this structure).
  - In the high temperature phase the samarium and barium sites may be disordered, in which case the system is in the cubic perovskite ($E2_1$) structure.

- Here we use the structural information from (Sagayama, 2019) at 400K.
- The cubic perovskite phase may be recovered from this structure by replacing the barium atoms by samarium, setting $a = b = c$, and setting all variable Wyckoff position parameters to $1/4$.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}}$	(4g)	Ba I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(4g)	Ba I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Sm I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Sm I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$by_3\,\hat{\mathbf{y}}$	(4i)	O I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-by_3\,\hat{\mathbf{y}}$	(4i)	O I
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	O II
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	O II
$\mathbf{B_9}$	=	$z_5\,\mathbf{a}_3$	=	$cz_5\,\hat{\mathbf{z}}$	(4k)	O III
$\mathbf{B_{10}}$	=	$-z_5\,\mathbf{a}_3$	=	$-cz_5\,\hat{\mathbf{z}}$	(4k)	O III
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4l)	O IV
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$	(4l)	O IV
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8m)	O V
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_7\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8m)	O V
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8m)	O V
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_7\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8m)	O V
$\mathbf{B_{17}}$	=	$-y_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8n)	Mn I
$\mathbf{B_{18}}$	=	$y_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8n)	Mn I
$\mathbf{B_{19}}$	=	$-y_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8n)	Mn I
$\mathbf{B_{20}}$	=	$y_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8n)	Mn I

References

[1] H. Sagayama, S. Toyoda, K. Sugimoto, Y. Maeda, S. Yamada, and T. Arima, *Ferroelectricity driven by charge ordering in the A-site ordered perovskite manganite $SmBaMn_2O_6$*, Phys. Rev. B **96**, 241113(R) (2014), doi:10.1103/PhysRevB.90.241113.

Found in

[1] L. Chen, Z. Xiang, C. Tinsman, Q. Huang, K. G. Reynolds, H. Zhou, and L. Li, *Anomalous thermal conductivity across the structural transition in* $SmBaMn_2O_6$ *single crystals*, Appl. Phys. Lett. **114**, 251904 (2019), doi:10.1063/1.5096960.