β-$K_2Bi_8Se_{13}$ Structure: A8B2C13_mP46_11_8e_2e_13e-001

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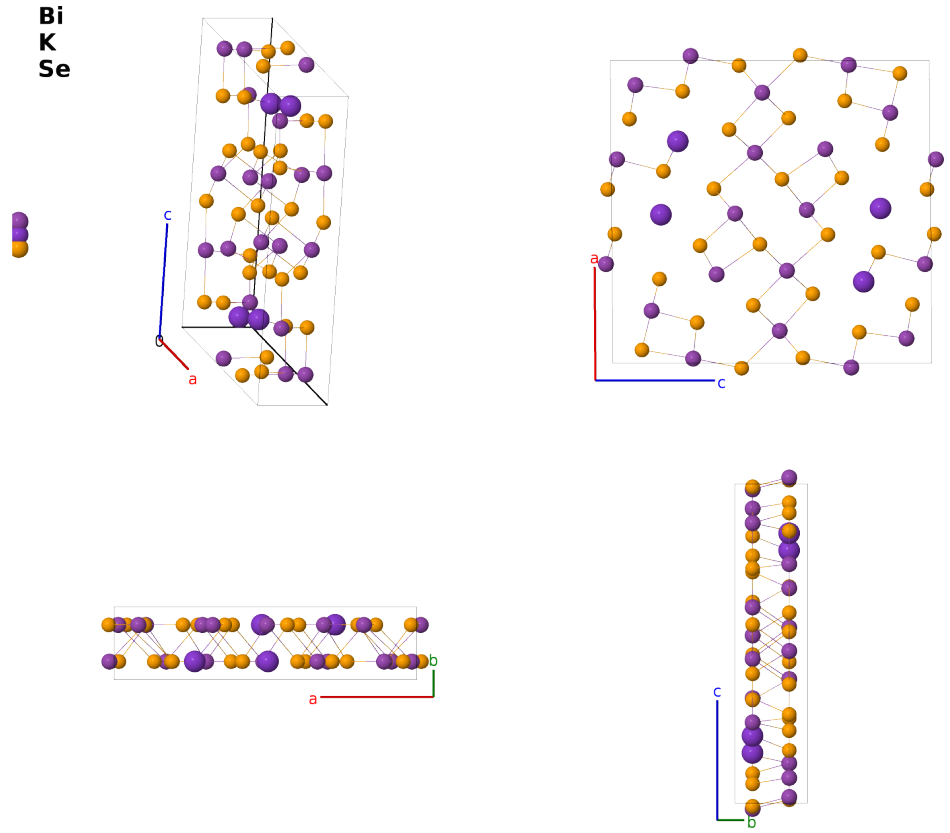
https://aflow.org/prototype-encyclopedia/68FX

https://aflow.org/prototype-encyclopedia/A8B2C13_mP46_11_8e_2e_13e-001



Prototype	$Bi_8K_2Se_{13}$
AFLOW prototype label	A8B2C13_mP46_11_8e_2e_13e-001
ICSD	84268
CCDC	1644272
Pearson symbol	mP46
Space group number	11
Space group symbol	$P2_1/m$
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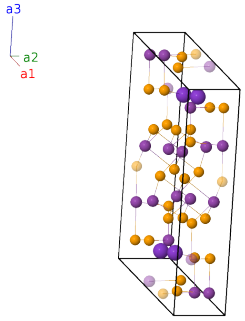
Other compounds with this structure
$Eu_4Bi_6Se_{13}$, $Sr_4Bi_6Se_{13}$

- The Bi VIII site is actually 62% bismuth and 38% potassium, while the K I site is 62% potassium and 38% bismuth.
- $K_2Bi_8Se_{13}$ can also be found in the triclinic α phase, which has no compositional disorder.

Simple Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= a\,\hat{\mathbf{x}} \\
\mathbf{a_2} &= b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi IV
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi IV
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi V
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi V
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi VI
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi VI
$\mathbf{B_{13}}$	=	$x_7\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi VII
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi VII
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi VIII
$\mathbf{B_{16}}$	=	$-x_8\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(2e)	Bi VIII
$\mathbf{B_{17}}$	=	$x_9\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(2e)	K I
$\mathbf{B_{18}}$	=	$-x_9\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(2e)	K I
$\mathbf{B_{19}}$	=	$x_{10}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2e)	K II
$\mathbf{B_{20}}$	=	$-x_{10}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2e)	K II
$\mathbf{B_{21}}$	=	$x_{11}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se I
$\mathbf{B_{22}}$	=	$-x_{11}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se I

$\mathbf{B_{23}}$	$=$	$x_{12}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	$=$	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se II
$\mathbf{B_{24}}$	$=$	$-x_{12}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se II
$\mathbf{B_{25}}$	$=$	$x_{13}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	$=$	$(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se III
$\mathbf{B_{26}}$	$=$	$-x_{13}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se III
$\mathbf{B_{27}}$	$=$	$x_{14}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	$=$	$(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se IV
$\mathbf{B_{28}}$	$=$	$-x_{14}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se IV
$\mathbf{B_{29}}$	$=$	$x_{15}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	$=$	$(ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se V
$\mathbf{B_{30}}$	$=$	$-x_{15}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	$=$	$-(ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se V
$\mathbf{B_{31}}$	$=$	$x_{16}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	$=$	$(ax_{16} + cz_{16}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se VI
$\mathbf{B_{32}}$	$=$	$-x_{16}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3$	$=$	$-(ax_{16} + cz_{16}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se VI
$\mathbf{B_{33}}$	$=$	$x_{17}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3$	$=$	$(ax_{17} + cz_{17}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se VII
$\mathbf{B_{34}}$	$=$	$-x_{17}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3$	$=$	$-(ax_{17} + cz_{17}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se VII
$\mathbf{B_{35}}$	$=$	$x_{18}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3$	$=$	$(ax_{18} + cz_{18}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se VIII
$\mathbf{B_{36}}$	$=$	$-x_{18}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3$	$=$	$-(ax_{18} + cz_{18}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se VIII
$\mathbf{B_{37}}$	$=$	$x_{19}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3$	$=$	$(ax_{19} + cz_{19}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se IX
$\mathbf{B_{38}}$	$=$	$-x_{19}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{19}\,\mathbf{a}_3$	$=$	$-(ax_{19} + cz_{19}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se IX
$\mathbf{B_{39}}$	$=$	$x_{20}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3$	$=$	$(ax_{20} + cz_{20}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{20}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se X
$\mathbf{B_{40}}$	$=$	$-x_{20}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{20}\,\mathbf{a}_3$	$=$	$-(ax_{20} + cz_{20}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{20}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se X
$\mathbf{B_{41}}$	$=$	$x_{21}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3$	$=$	$(ax_{21} + cz_{21}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{21}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se XI
$\mathbf{B_{42}}$	$=$	$-x_{21}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{21}\,\mathbf{a}_3$	$=$	$-(ax_{21} + cz_{21}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{21}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se XI
$\mathbf{B_{43}}$	$=$	$x_{22}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{22}\,\mathbf{a}_3$	$=$	$(ax_{22} + cz_{22}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{22}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se XII
$\mathbf{B_{44}}$	$=$	$-x_{22}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{22}\,\mathbf{a}_3$	$=$	$-(ax_{22} + cz_{22}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{22}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se XII
$\mathbf{B_{45}}$	$=$	$x_{23}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_{23}\,\mathbf{a}_3$	$=$	$(ax_{23} + cz_{23}\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_{23}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se XIII
$\mathbf{B_{46}}$	$=$	$-x_{23}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_{23}\,\mathbf{a}_3$	$=$	$-(ax_{23} + cz_{23}\cos\beta)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_{23}\sin\beta\,\hat{\mathbf{z}}$	(2e)	Se XIII

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[1] D.-Y. Chung, K.-S. Choi, L. Iordanidis, J. L. Schindler, P. W. Brazis, C. R. Kannewurf, B. Chen, S. Hu, C. Uher, and M. G. Kanatzidis, *High Thermopower and Low Thermal Conductivity in Semiconducting Ternary K-Bi-Se Compounds. Synthesis and Properties of β-$K_2Bi_8Se_{13}$ and $K_{2.5}Bi_{8.5}Se_{14}$ and Their Sb Analogues*, Chem. Mater. **9**, 3060–3067 (1997), doi:10.1021/cm970397e.

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