

Synthesis, Crystal Structure, and Thermoelectric Properties of Two New Barium Antimony Selenides: $\text{Ba}_2\text{Sb}_2\text{Se}_5$ and $\text{Ba}_6\text{Sb}_7\text{Se}_{16.11}$

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Supporting Information

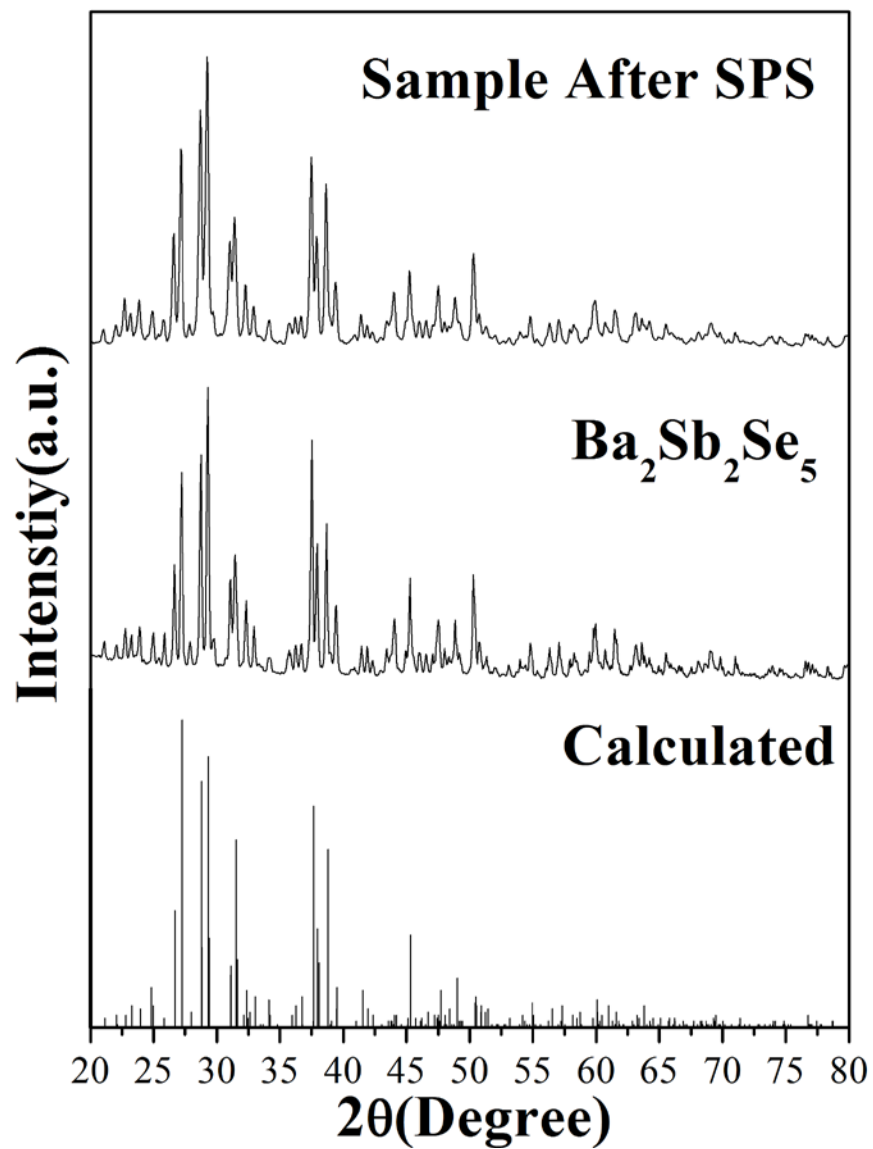


Figure S1. Powder X-ray diffraction patterns of Ba₂Sb₂Se₅ before (middle) and after (top) the SPS process. Calculated pattern is shown on the bottom.

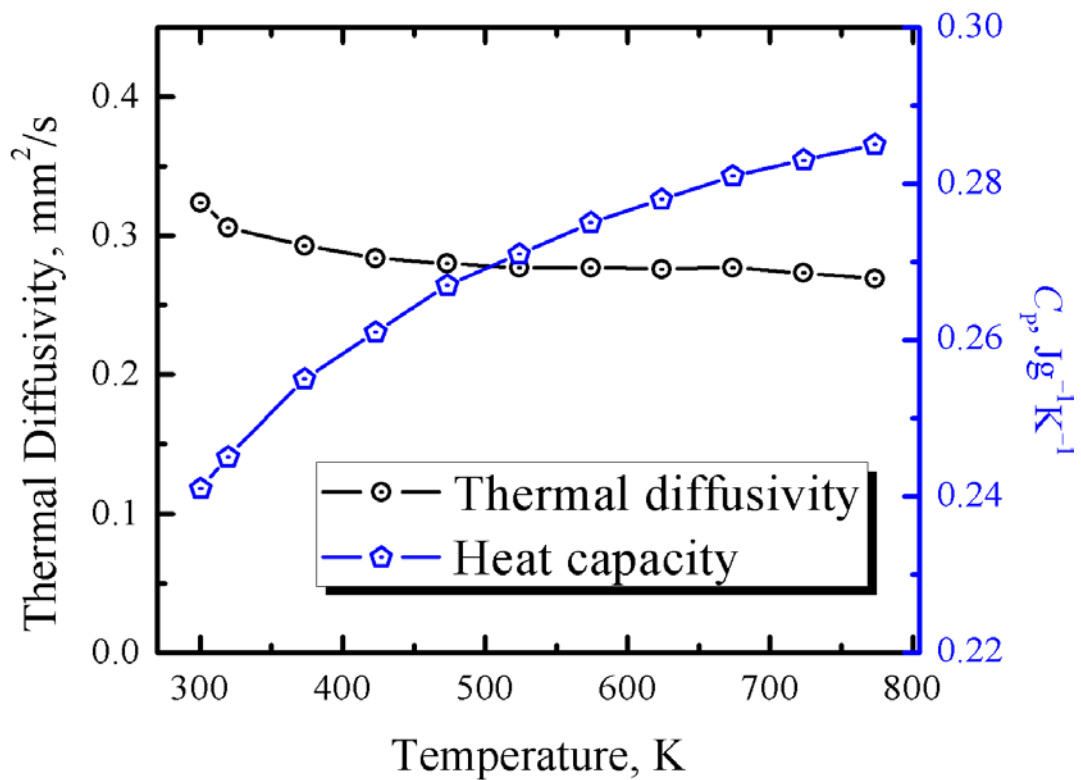


Figure S2. Temperature dependences of the thermal diffusivity (black) and heat capacity (blue) for Ba₂Sb₂Se₅.

Table S1. EDX spectroscopy results for selected samples of $\text{Ba}_2\text{Sb}_2\text{Se}_5$. The compositions were normalized to 2 Sb atoms.

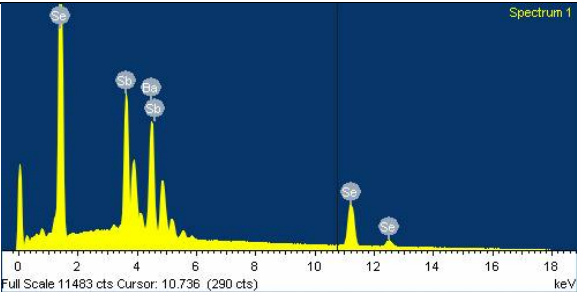
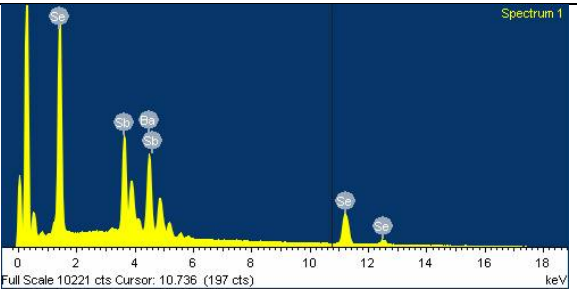
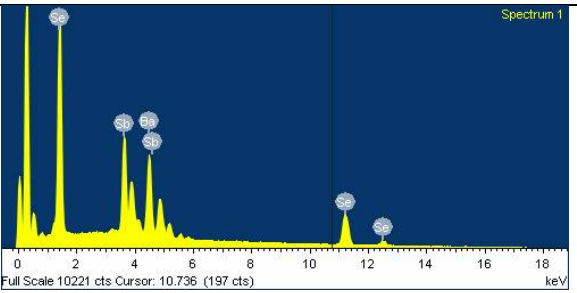
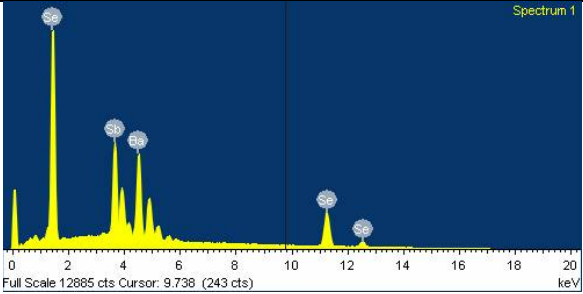
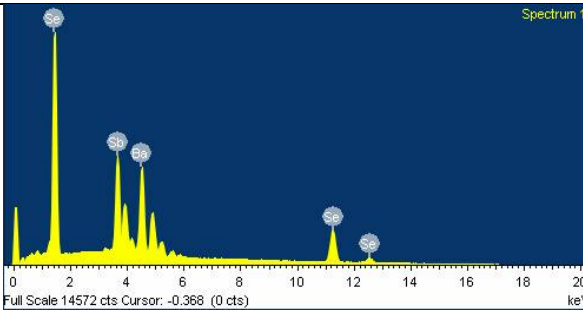
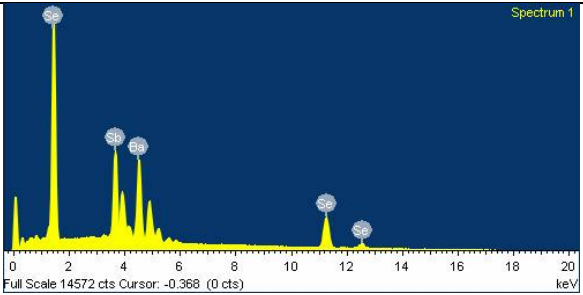
Spectrum	Composition
 <p>Full Scale 11483 cts Cursor: 10.736 (290 cts)</p>	$\text{Ba}_{2.03}\text{Sb}_2\text{Se}_{4.94}$
 <p>Full Scale 10221 cts Cursor: 10.736 (197 cts)</p>	$\text{Ba}_{1.99}\text{Sb}_2\text{Se}_{4.77}$
 <p>Full Scale 10221 cts Cursor: 10.736 (197 cts)</p>	$\text{Ba}_{2.01}\text{Sb}_2\text{Se}_{4.99}$

Table S2. EDX spectroscopy results for selected samples of $\text{Ba}_6\text{Sb}_7\text{Se}_{16.11}$. The compositions were normalized to 7 Sb atoms. The admixtures contained in the samples prevent accurate composition determination.

Spectrum	Composition
 <p>Full Scale 12885 cts Cursor: 9.738 (243 cts)</p>	$\text{Ba}_{7.85}\text{Sb}_7\text{Se}_{17.1}$
 <p>Full Scale 14572 cts Cursor: -0.368 (0 cts)</p>	$\text{Ba}_{7.93}\text{Sb}_7\text{Se}_{17.8}$
 <p>Full Scale 14572 cts Cursor: -0.368 (0 cts)</p>	$\text{Ba}_{7.78}\text{Sb}_7\text{Se}_{18.7}$

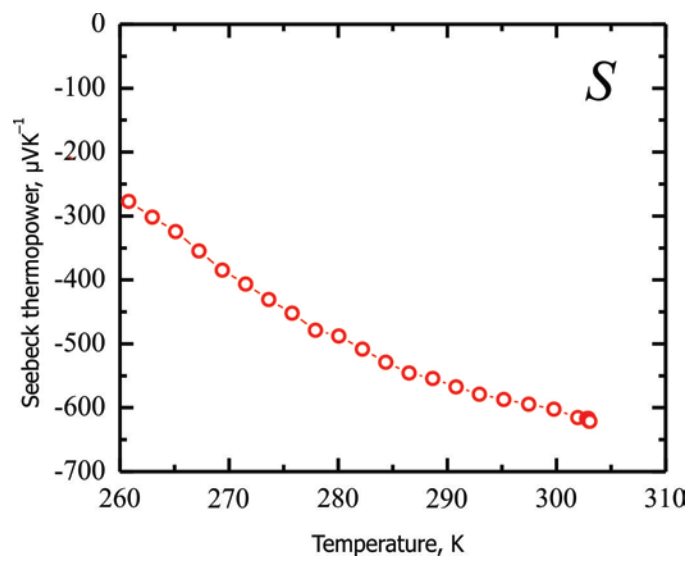


Figure S3. Temperature dependence of the Seebeck thermopower of $\text{Ba}_2\text{Sb}_2\text{Se}_5$.

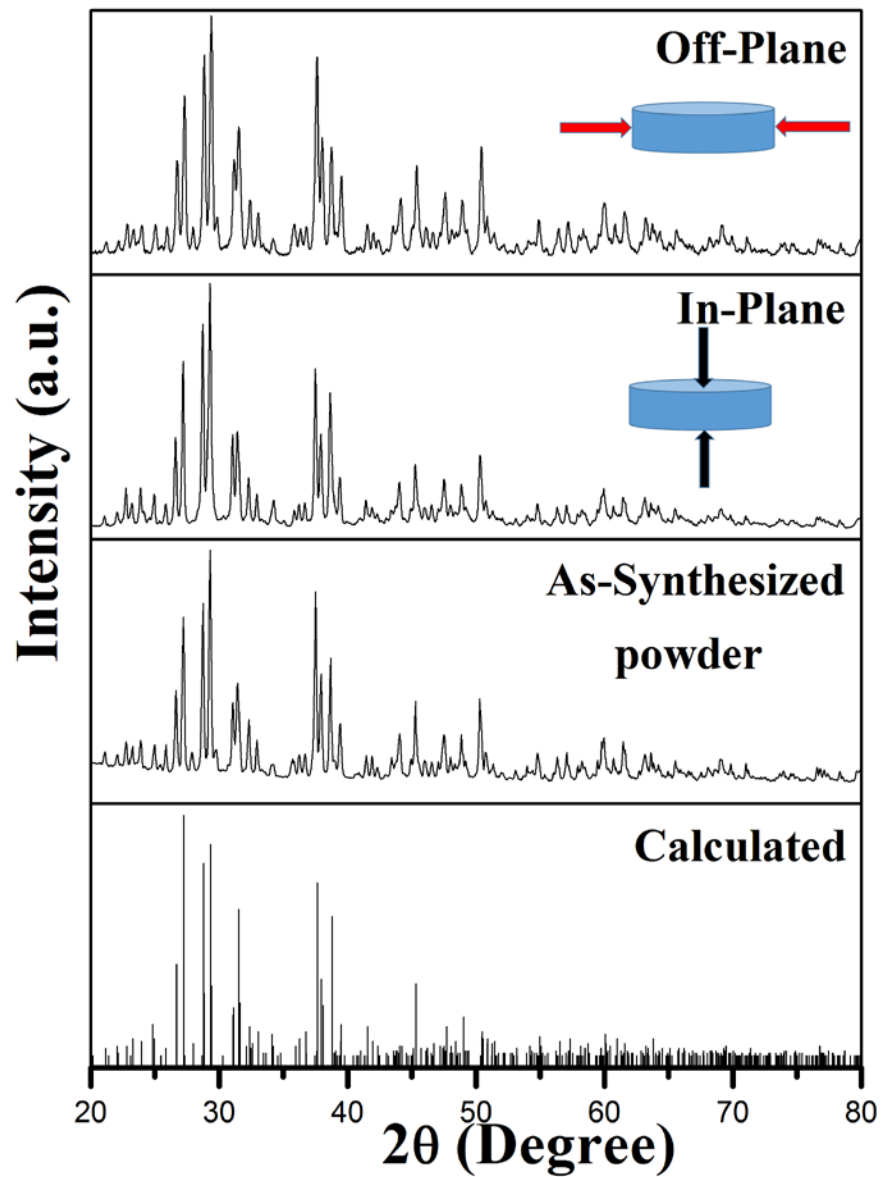


Figure S4. Powder X-ray diffraction patterns of $\text{Ba}_2\text{Sb}_2\text{Se}_5$ SPS-pellet measured off-plane (top) and in-plane (middle). Calculated pattern is shown on the bottom.