

Low-temperature solution route for the synthesis of single crystals of BaSe_3 and its photovoltaic study

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Electronic Supplementary Information (ESI)

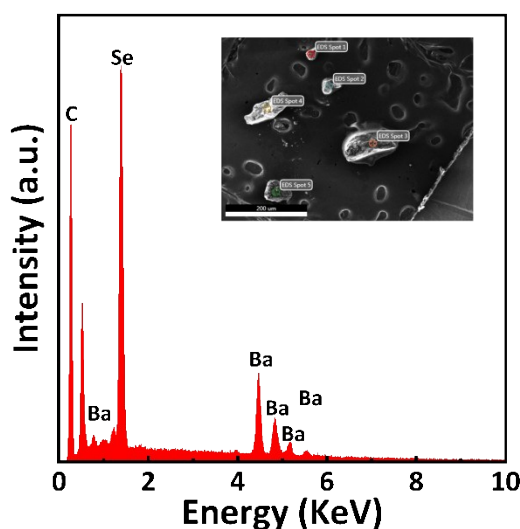


Fig. S11: The EDX spectrum of a BaSe_3 crystal. The inset shows an FE-SEM image of a few BaSe_3 crystals. These data were collected with the help of a field emission scanning electron microscope equipped with an octane elite (EDX Inc, USA) spectrometer.

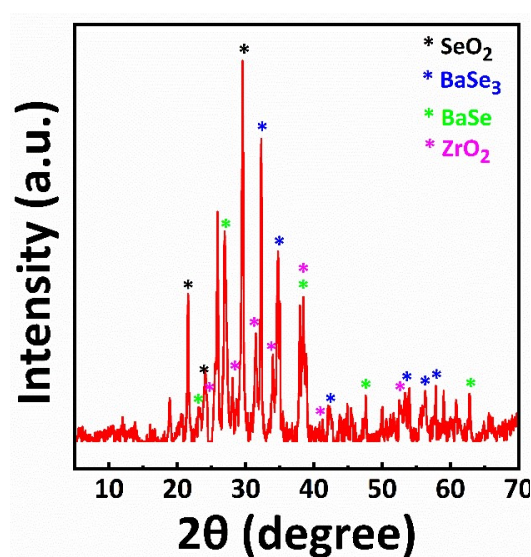


Fig. S12: The PXR D pattern of the precipitate left after dissolving $\text{Ba}_8\text{Zr}_2\text{Se}_{11}(\text{Se}_2)$ in water.

Table SI1: The atomic displacement parameters (\AA^2) for the BaSe_3 structure.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.01483 (15)	0.01483 (15)	0.0123 (2)	0.000	0.000	0.000
Se1	0.01116 (16)	0.01116 (16)	0.0178 (3)	0.00006 (19)	-0.00055 (17)	-0.00055 (17)
Se2	0.0121 (2)	0.0121 (2)	0.0160 (4)	-0.0004 (3)	0.000	0.000

Table SI2: The bond angles for the BaSe_3 structure.

Se1 ⁱ –Ba1–Se1 ⁱⁱ	112.101 (9)	Se1 ⁱⁱ –Ba1–Se2 ^{ix}	122.062 (10)
Se1 ⁱ –Ba1–Se1 ⁱⁱⁱ	104.332 (17)	Se1 ⁱⁱⁱ –Ba1–Se2 ^{ix}	38.860 (12)
Se1 ⁱⁱ –Ba1–Se1 ⁱⁱⁱ	112.101 (9)	Se1 ^{iv} –Ba1–Se2 ^{ix}	73.282 (12)
Se1 ⁱ –Ba1–Se1 ^{iv}	112.101 (9)	Se1 ^v –Ba1–Se2 ^{ix}	59.117 (13)
Se1 ⁱⁱ –Ba1–Se1 ^{iv}	104.332 (17)	Se1 ^{vi} –Ba1–Se2 ^{ix}	58.315 (11)
Se1 ⁱⁱⁱ –Ba1–Se1 ^{iv}	112.101 (9)	Se1 ^{vii} –Ba1–Se2 ^{ix}	140.052 (13)
Se1 ⁱ –Ba1–Se1 ^v	178.116 (16)	Se1 ^{viii} –Ba1–Se2 ^{ix}	105.778 (11)
Se1 ⁱⁱ –Ba1–Se1 ^v	66.924 (3)	Se2 ⁱ –Ba1–Se2 ^{ix}	157.13 (2)
Se1 ⁱⁱⁱ –Ba1–Se1 ^v	77.552 (5)	Se2–Ba1–Se2 ^{ix}	92.252 (4)
Se1 ^{iv} –Ba1–Se1 ^v	66.924 (3)	Se1 ⁱ –Ba1–Se2 ^{iv}	73.282 (12)
Se1 ⁱ –Ba1–Se1 ^{vi}	66.924 (3)	Se1 ⁱⁱ –Ba1–Se2 ^{iv}	122.378 (13)
Se1 ⁱⁱ –Ba1–Se1 ^{vi}	178.116 (16)	Se1 ⁱⁱⁱ –Ba1–Se2 ^{iv}	122.062 (11)
Se1 ⁱⁱⁱ –Ba1–Se1 ^{vi}	66.924 (3)	Se1 ^{iv} –Ba1–Se2 ^{iv}	38.860 (12)
Se1 ^{iv} –Ba1–Se1 ^{vi}	77.552 (5)	Se1 ^v –Ba1–Se2 ^{iv}	105.778 (12)
Se1 ^v –Ba1–Se1 ^{vi}	114.100 (9)	Se1 ^{vi} –Ba1–Se2 ^{iv}	59.117 (13)
Se1 ⁱ –Ba1–Se1 ^{vii}	77.552 (5)	Se1 ^{vii} –Ba1–Se2 ^{iv}	58.315 (11)
Se1 ⁱⁱ –Ba1–Se1 ^{vii}	66.924 (3)	Se1 ^{viii} –Ba1–Se2 ^{iv}	140.052 (13)
Se1 ⁱⁱⁱ –Ba1–Se1 ^{vii}	178.116 (16)	Se2 ⁱ –Ba1–Se2 ^{iv}	92.252 (4)
Se1 ^{iv} –Ba1–Se1 ^{vii}	66.924 (3)	Se2–Ba1–Se2 ^{iv}	157.13 (2)
Se1 ^v –Ba1–Se1 ^{vii}	100.564 (16)	Se2 ^{ix} –Ba1–Se2 ^{iv}	92.252 (4)
Se1 ^{vi} –Ba1–Se1 ^{vii}	114.100 (9)	Se2–Se1–Ba1 ^x	78.974 (16)
Se1 ⁱ –Ba1–Se1 ^{viii}	66.924 (3)	Se2–Se1–Ba1 ^{xi}	78.974 (16)
Se1 ⁱⁱ –Ba1–Se1 ^{viii}	77.552 (5)	Ba1 ^x –Se1–Ba1 ^{xi}	100.579 (16)
Se1 ⁱⁱⁱ –Ba1–Se1 ^{viii}	66.924 (3)	Se2–Se1–Ba1 ^{xii}	119.948 (13)
Se1 ^{iv} –Ba1–Se1 ^{viii}	178.116 (16)	Ba1 ^x –Se1–Ba1 ^{xii}	77.552 (5)
Se1 ^v –Ba1–Se1 ^{viii}	114.100 (9)	Ba1 ^{xi} –Se1–Ba1 ^{xii}	159.584 (17)
Se1 ^{vi} –Ba1–Se1 ^{viii}	100.564 (16)	Se2–Se1–Ba1 ^{xiii}	119.948 (13)

Se1 ^{vii} –Ba1–Se1 ^{viii}	114.100 (9)	Ba1 ^x –Se1–Ba1 ^{xiii}	159.584 (17)
Se1 ⁱ –Ba1–Se2 ⁱ	38.860 (12)	Ba1 ^{xi} –Se1–Ba1 ^{xiii}	77.552 (5)
Se1 ⁱⁱ –Ba1–Se2 ⁱ	73.282 (12)	Ba1 ^{xii} –Se1–Ba1 ^{xiii}	97.048 (16)
Se1 ⁱⁱⁱ –Ba1–Se2 ⁱ	122.378 (13)	Se1–Se2–Se1 ⁱⁱ	112.66 (4)
Se1 ^{iv} –Ba1–Se2 ⁱ	122.062 (11)	Se1–Se2–Ba1	133.370 (12)
Se1 ^v –Ba1–Se2 ⁱ	140.052 (13)	Se1 ⁱⁱ –Se2–Ba1	62.166 (9)
Se1 ^{vi} –Ba1–Se2 ⁱ	105.778 (11)	Se1–Se2–Ba1 ^{xiv}	133.370 (12)
Se1 ^{vii} –Ba1–Se2 ⁱ	59.117 (13)	Se1 ⁱⁱ –Se2–Ba1 ^{xiv}	62.166 (9)
Se1 ^{viii} –Ba1–Se2 ⁱ	58.315 (11)	Ba1–Se2–Ba1 ^{xiv}	87.748 (4)
Se1 ⁱ –Ba1–Se2	122.062 (10)	Se1–Se2–Ba1 ^{xi}	62.167 (9)
Se1 ⁱⁱ –Ba1–Se2	38.860 (12)	Se1 ⁱⁱ –Se2–Ba1 ^{xi}	133.370 (12)
Se1 ⁱⁱⁱ –Ba1–Se2	73.282 (12)	Ba1–Se2–Ba1 ^{xi}	157.13 (2)
Se1 ^{iv} –Ba1–Se2	122.378 (13)	Ba1 ^{xiv} –Se2–Ba1 ^{xi}	87.748 (4)
Se1 ^v –Ba1–Se2	58.315 (11)	Se1–Se2–Ba1 ^x	62.167 (9)
Se1 ^{vi} –Ba1–Se2	140.052 (13)	Se1 ⁱⁱ –Se2–Ba1 ^x	133.370 (12)
Se1 ^{vii} –Ba1–Se2	105.778 (11)	Ba1–Se2–Ba1 ^x	87.748 (4)
Se1 ^{viii} –Ba1–Se2	59.117 (13)	Ba1 ^{xiv} –Se2–Ba1 ^x	157.13 (2)
Se2 ⁱ –Ba1–Se2	92.252 (4)	Ba1 ^{xi} –Se2–Ba1 ^x	87.748 (4)
Se1 ⁱ –Ba1–Se2 ^{ix}	122.378 (13)		

Symmetry codes: (i) $y-1, -x, -z$; (ii) $-x, -y+1, z$; (iii) $-y+1, x, -z$; (iv) $x, y-1, z$; (v) $-y+1, x, -z+1$; (vi) $x, y-1, z-1$; (vii) $y-1, -x, -z+1$; (viii) $-x, -y+1, z-1$; (ix) $y, -x, -z$; (x) $x+1/2, -y+1/2, -z$; (xi) $x, y+1, z$; (xii) $x+1/2, -y+1/2, -z+1$; (xiii) $x, y+1, z+1$; (xiv) $x-1/2, -y+1/2, -z$.