

Supporting Information

BaZnBe₂(BO₃)₂F₂: a novel zinc-beryllium borate with SBBO-type structure overcoming the polymorphism problem

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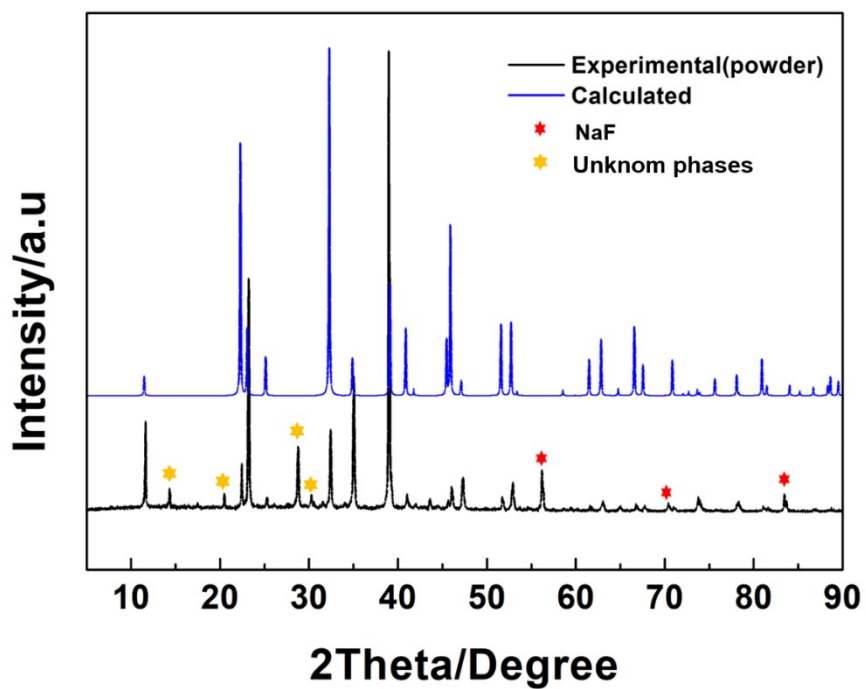


Figure S1. Powder XRD patterns of $\text{BaZnBe}_2(\text{BO}_3)_2\text{F}_2$.

As shown in Figure S1, the XRD data measured by the polycrystal powders is roughly consistent with the calculated curve from the CIF data. (Unfortunately, the pure phase has been attempted many times, without success.) There are some extra peaks which are from the raw material of NaF, and four peaks of unknown phases.

Table S1. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for $\text{BaZnBe}_2(\text{BO}_3)_2\text{F}_2$.

BaZnBe₂(BO₃)₂F₂				
Atom	x	y	z	U(eq)
Zn	0.0000	-1.0000	0.0000	0.0055 (3)
O1	-0.3488 (7)	-0.9730 (7)	-0.1728 (4)	0.0059 (6)
F1	0.3333	-0.3333	0.1728 (10)	0.0035 (10)
B1	-0.6667	-1.3333	-0.4353 (5)	0.0082 (7)
Ba	0.0000	-1.0000	0.5000	0.0083 (2)
Be1	-0.6667	-1.3333	-0.2256 (11)	-0.0017(10)

Table S2. Anisotropic displacement parameters (\AA^2) for $\text{BaZnBe}_2(\text{BO}_3)_2\text{F}_2$.

BaZnBe₂(BO₃)₂F₂						
Atom	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Zn	0.0053 (3)	0.0053 (3)	0.0060 (5)	0.00266(17)	0.000	0.000
O1	0.0053 (9)	0.0048 (9)	0.0081 (10)	0.0030 (7)	-0.0014 (7)	-0.0008 (7)
F1	0.0039 (10)	0.0039 (10)	0.0029 (14)	0.0019 (5)	0.000	0.000
B1	0.0083 (7)	0.0083 (7)	0.0080 (11)	0.0041 (4)	0.000	0.000
Ba	0.0070 (3)	0.0070 (3)	0.0109 (3)	0.00352(13)	0.000	0.000
Be1	0.0016 (10)	0.0016 (10)	0.0018 (14)	0.0008 (5)	0.000	0.000

Table S3. Selected bond lengths (Å) for BaZnBe₂(BO₃)₂F₂.

BaZnBe₂(BO₃)₂F₂			
Zn-O1	2.136 (3)	Ba-O1 ^v	3.024 (3)
Zn-O1 ⁱ	2.136 (3)	Ba-O1 ⁱⁱ	3.024 (3)
Zn-O1 ⁱⁱ	2.136 (3)	Ba-O1 ^{xi}	3.024 (3)
Zn-O1 ⁱⁱⁱ	2.136 (3)	Ba-O1 ⁱⁱⁱ	3.024 (3)
Zn-O1 ^{iv}	2.136 (3)	Ba-O1 ^{xii}	3.024 (3)
Zn-O1 ^v	2.136 (3)	Ba-O1 ^{xiii}	3.024 (3)
Zn-Ba ^{vi}	3.8518 (5)	Ba-F1 ^{xiv}	2.7020 (8)
Zn-Ba	3.8518 (5)	Ba-F1 ^{xii}	2.7020 (8)
O1-B1 ^{vii}	1.375 (3)	Ba-F1 ^{xv}	2.7020 (8)
O1-Ba ^{vi}	3.024 (3)	Ba-F1 ^{xvi}	2.7020 (8)
O1-Be1	1.621 (3)	Ba-F1 ^{xvii}	2.7020 (8)
B1-O1 ^{viii}	1.375 (3)	Ba-F1 ^v	2.7020 (8)
B1-O1 ⁱⁱⁱ	1.375 (3)	Be1-O1 ^{xviii}	1.621 (3)
B1-O1 ^{vii}	1.375 (3)	Be1-O1 ^{xix}	1.621 (3)
F1-Ba ^{ix}	2.7020 (8)	Be1-Ba ^{vi}	3.394 (5)
F1-Ba ^x	2.7020 (8)	Be1-Ba ^x	3.394 (5)
F1-Ba ^{vi}	2.7020 (8)	Be1-Ba ^{ix}	3.394 (5)
F1-Be1	1.615 (9)		

Symmetry codes: (i) $-x+y+1, -x-1, z$; (ii) $x-y-1, x-1, -z$; (iii) $y+1, -x+y, -z$; (iv) $-y-1, x-y-2, z$; (v) $-x, -y-2, -z$; (vi) $x, y, z-1$; (vii) $-x, -y-1, -z$; (viii) $x-y, x, -z$; (ix) $x-1, y, z-1$; (x) $x-1, y-1, z-1$; (xi) $-y-1, x-y-2, z+1$; (xii) $x, y, z+1$; (xiii) $-x+y+1, -x-1, z+1$; (xiv) $-x-1, -y-2, -z$; (xv) $x+1, y+1, z+1$; (xvi) $x+1, y, z+1$; (xvii) $-x-1, -y-3, -z$; (xviii) $-y-2, x-y-2, z$; (xix) $-x+y, -x-2, z$.

Table S4. Selected bond angles (degree) for BaZnBe₂(BO₃)₂F₂.

O1-Zn-O1 ⁱⁱⁱ	94.75 (11)	F1 ^{xii} -Ba-O1 ^{xii}	52.74 (9)
O1 ^{iv} -Zn-O1 ⁱⁱ	94.75 (11)	F1 ^v -Ba-O1 ^{xi}	100.87 (9)
O1 ^v -Zn-O1 ⁱ	94.75 (11)	F1 ^{xvi} -Ba-O1 ⁱⁱ	100.87 (9)
O1-Zn-O1 ^{iv}	85.25 (11)	F1 ^{xvii} -Ba-O1 ^{xiii}	127.26 (9)
O1-Zn-O1 ⁱ	85.25 (11)	F1 ^{xvii} -Ba-O1 ⁱⁱ	52.74 (9)
O1 ⁱⁱⁱ -Zn-O1 ^{iv}	180.00 (11)	F1 ^{xvii} -Ba-O1 ⁱⁱⁱ	109.45 (10)
O1 ⁱⁱⁱ -Zn-O1 ⁱⁱ	85.25 (11)	F1 ^{xiv} -Ba-O1 ^v	109.45 (10)
O1-Zn-O1 ^v	180.0	F1 ^v -Ba-O1 ^{xiii}	70.55 (10)
O1 ^v -Zn-O1 ⁱⁱ	85.25 (11)	F1 ^{xvi} -Ba-O1 ^v	70.55 (10)
O1 ⁱⁱⁱ -Zn-O1 ^v	85.25 (11)	F1 ^{xvi} -Ba-O1 ^{xii}	109.45 (10)
O1 ⁱⁱⁱ -Zn-O1 ⁱ	94.75 (11)	F1 ^{xv} -Ba-O1 ^v	100.87 (9)
O1 ^{iv} -Zn-O1 ^v	94.75 (11)	F1 ^{xii} -Ba-O1 ^{xi}	79.13 (9)
O1 ⁱⁱ -Zn-O1 ⁱ	180.0	F1 ^v -Ba-O1 ^v	52.74 (9)
O1-Zn-O1 ⁱⁱ	94.75 (11)	F1 ^{xvi} -Ba-O1 ^{xiii}	79.13 (9)
O1 ^{iv} -Zn-O1 ⁱ	85.25 (11)	F1 ^{xii} -Ba-O1 ^v	127.26 (10)
O1-Zn-Ba ^{vi}	51.44 (7)	F1 ^{xv} -Ba-O1 ^{xiii}	52.74 (9)
O1 ^v -Zn-Ba	51.44 (7)	F1 ^{xv} -Ba-O1 ⁱⁱ	127.26 (9)
O1 ⁱⁱⁱ -Zn-Ba	51.44 (7)	F1 ^{xvi} -Ba-O1 ⁱⁱⁱ	127.26 (9)
O1 ^{iv} -Zn-Ba ^{vi}	51.44 (7)	F1 ^v -Ba-O1 ⁱⁱ	109.45 (10)
O1-Zn-O1 ⁱⁱⁱ	94.75 (11)	F1 ^{xii} -Ba-O1 ^{xii}	52.74 (9)
O1 ^{iv} -Zn-O1 ⁱⁱ	94.75 (11)	F1 ^v -Ba-O1 ^{xi}	100.87 (9)
O1 ^v -Zn-O1 ⁱ	94.75 (11)	F1 ^{xvi} -Ba-O1 ⁱⁱ	100.87 (9)
O1-Zn-O1 ^{iv}	85.25 (11)	F1 ^{xvii} -Ba-O1 ^{xiii}	127.26 (9)
O1-Zn-O1 ⁱ	85.25 (11)	F1 ^{xvii} -Ba-O1 ⁱⁱ	52.74 (9)
O1 ⁱⁱⁱ -Zn-O1 ^{iv}	180.00 (11)	F1 ^{xvii} -Ba-O1 ⁱⁱⁱ	109.45 (10)
O1 ⁱⁱⁱ -Zn-O1 ⁱⁱ	85.25 (11)	F1 ^{xiv} -Ba-O1 ^v	109.45 (10)
O1-Zn-O1 ^v	180.0	F1 ^v -Ba-O1 ^{xiii}	70.55 (10)
O1 ^v -Zn-O1 ⁱⁱ	85.25 (11)	F1 ^{xvi} -Ba-O1 ^v	70.55 (10)
O1 ⁱⁱⁱ -Zn-O1 ^v	85.25 (11)	F1 ^{xvi} -Ba-O1 ^{xii}	109.45 (10)
O1 ⁱⁱⁱ -Zn-O1 ⁱ	94.75 (11)	F1 ^{xv} -Ba-O1 ^v	100.87 (9)
O1 ^{iv} -Zn-O1 ^v	94.75 (11)	F1 ^{xii} -Ba-O1 ^{xi}	79.13 (9)
O1 ⁱⁱ -Zn-O1 ⁱ	180.0	F1 ^v -Ba-O1 ^v	52.74 (9)
O1-Zn-O1 ⁱⁱ	94.75 (11)	F1 ^{xvi} -Ba-O1 ^{xiii}	79.13 (9)
O1 ^{iv} -Zn-O1 ⁱ	85.25 (11)	F1 ^{xii} -Ba-O1 ^v	127.26 (10)
O1-Zn-Ba ^{vi}	51.44 (7)	F1 ^{xv} -Ba-O1 ^{xiii}	52.74 (9)
O1 ^v -Zn-Ba	51.44 (7)	F1 ^{xv} -Ba-O1 ⁱⁱ	127.26 (9)
O1 ⁱⁱⁱ -Zn-Ba	51.44 (7)	F1 ^{xvi} -Ba-O1 ⁱⁱⁱ	127.26 (9)
O1 ^{iv} -Zn-Ba ^{vi}	51.44 (7)	F1 ^v -Ba-O1 ⁱⁱ	109.45 (10)
O1 ⁱ -Zn-Ba	128.56 (7)	F1 ^{xv} -Ba-O1 ⁱⁱⁱ	70.55 (10)
O1 ^v -Zn-Ba ^{vi}	128.56 (7)	F1 ^{xii} -Ba-O1 ⁱⁱ	70.55 (10)
O1 ^{iv} -Zn-Ba	128.56 (7)	F1 ^{xii} -Ba-O1 ⁱⁱⁱ	100.87 (9)
O1 ⁱⁱ -Zn-Ba ^{vi}	128.56 (7)	F1 ^{xiv} -Ba-O1 ^{xi}	127.26 (9)
O1 ⁱⁱ -Zn-Ba	51.44 (7)	F1 ^{xii} -Ba-O1 ^{xiii}	109.45 (10)

O1 ⁱ -Zn-Ba ^{vi}	51.44 (7)	F1 ^{xvi} -Ba-O1 ^{xi}	52.74 (9)
O1-Zn-Ba	128.56 (7)	F1 ^{xiv} -Ba-O1 ^{xii}	70.55 (10)
O1 ⁱⁱⁱ -Zn-Ba ^{vi}	128.56 (7)	F1 ^{xvii} -Ba-O1 ^{xi}	70.55 (10)
Ba ^{vi} -Zn-Ba	180.0	F1 ^{xv} -Ba-O1 ^{xi}	109.45 (10)
Zn-O1-Ba ^{vi}	95.03 (9)	F1 ^{xvii} -Ba-O1 ^v	79.13 (9)
B1 ^{vii} -O1-Zn	113.8 (3)	F1 ^{xvii} -Ba-F1 ^{xv}	180.00 (17)
B1 ^{vii} -O1-Ba ^{vi}	106.6 (3)	F1 ^v -Ba-F1 ^{xii}	180.0
B1 ^{vii} -O1-Be1	127.3 (2)	F1 ^{xiv} -Ba-F1 ^{xv}	63.32 (5)
Be1-O1-Zn	114.6 (2)	F1 ^{xiv} -Ba-F1 ^v	116.68 (5)
Be1-O1-Ba ^{vi}	88.5 (3)	F1 ^{xiv} -Ba-F1 ^{xvii}	116.68 (5)
O1 ^{vii} -B1-O1 ⁱⁱⁱ	120.000 (1)	F1 ^{xvi} -Ba-F1 ^v	63.32 (5)
O1 ^{vii} -B1-O1 ^{viii}	120.000 (1)	F1 ^{xvii} -Ba-F1 ^{xii}	63.32 (5)
O1 ⁱⁱⁱ -B1-O1 ^{viii}	120.000 (1)	F1 ^{xvii} -Ba-F1 ^v	116.68 (5)
Ba ^{ix} -F1-Ba ^{vi}	116.68 (5)	F1 ^{xiv} -Ba-F1 ^{xvi}	180.0
Ba ^{ix} -F1-Ba ^x	116.68 (5)	F1 ^{xv} -Ba-F1 ^v	63.32 (5)
Ba ^x -F1-Ba ^{vi}	116.68 (5)	F1 ^{xvi} -Ba-F1 ^{xvii}	63.32 (5)
Be1-F1-Ba ^x	100.62 (9)	F1 ^{xiv} -Ba-F1 ^{xii}	63.32 (5)
Be1-F1-Ba ^{ix}	100.62 (9)	F1 ^{xvi} -Ba-F1 ^{xv}	116.68 (5)
Be1-F1-Ba ^{vi}	100.62 (9)	F1 ^{xvi} -Ba-F1 ^{xii}	116.68 (5)
O1 ^v -Ba-O1 ^{xi}	122.84 (8)	F1 ^{xv} -Ba-F1 ^{xii}	116.68 (5)
O1 ^{xiii} -Ba-O1 ^v	122.84 (8)	O1 ^{xviii} -Be1-O1 ^{xix}	113.9 (2)
O1 ^{xiii} -Ba-O1 ^{xi}	57.16 (8)	O1-Be1-O1 ^{xix}	113.9 (2)
O1 ^{xii} -Ba-O1 ^v	180.00 (11)	O1 ^{xviii} -Be1-O1	113.9 (2)
O1 ^v -Ba-O1 ⁱⁱⁱ	57.16 (8)	O1 ^{xviii} -Be1-Ba ^{ix}	62.94 (19)
O1 ⁱⁱ -Ba-O1 ^{xi}	122.84 (8)	O1 ^{xix} -Be1-Ba ^x	62.94 (19)
O1 ^{xiii} -Ba-O1 ⁱⁱⁱ	122.84 (8)	O1-Be1-Ba ^{vi}	62.95 (19)
O1 ^{xii} -Ba-O1 ^{xi}	57.16 (8)	O1-Be1-Ba ^{ix}	94.28 (18)
O1 ⁱⁱ -Ba-O1 ^v	57.16 (8)	O1 ^{xviii} -Be1-Ba ^{vi}	148.1 (3)
O1 ⁱⁱ -Ba-O1 ⁱⁱⁱ	57.16 (8)	O1 ^{xix} -Be1-Ba ^{ix}	148.1 (3)
O1 ⁱⁱ -Ba-O1 ^{xiii}	180.00 (6)	O1 ^{xix} -Be1-Ba ^{vi}	94.28 (18)
O1 ^{xii} -Ba-O1 ⁱⁱⁱ	122.84 (8)	O1-Be1-Ba _x	148.1 (3)
O1 ⁱⁱ -Ba-O1 ^{xii}	122.84 (8)	O1 ^{xviii} -Be1-Ba _x	94.28 (18)
O1 ^{xi} -Ba-O1 ⁱⁱⁱ	180.00 (11)	F1-Be1-O1 _{xix}	104.5 (3)
O1 ^{xiii} -Ba-O1 ^{xii}	57.16 (8)	F1-Be1-O1	104.5 (3)
F1 ^{xvii} -Ba-O1 ^{xii}	100.87 (9)	F1-Be1-O1 ^{xviii}	104.5 (3)
F1 ^{xiv} -Ba-O1 ⁱⁱ	79.13 (9)	F1-Be1-Ba _{vi}	51.49 (11)
F1 ^{xiv} -Ba-O1 ⁱⁱⁱ	52.74 (9)	F1-Be1-Ba _x	51.49 (11)
F1 ^{xv} -Ba-O1 ^{xii}	79.13 (9)	F1-Be1-Ba _{ix}	51.49 (11)
F1 ^{xiv} -Ba-O1 ^{xiii}	100.87 (9)	Ba _x -Be1-Ba _{vi}	85.32 (16)
F1 ^v -Ba-O1 ^{xii}	127.26 (9)	Ba _{ix} -Be1-Ba _x	85.32 (16)
F1 ^v -Ba-O1 ⁱⁱⁱ	79.13 (9)	Ba _{ix} -Be1-Ba _{vi}	85.32 (16)
Zn-O1-Be1-O1 ^{xix}	-12.6 (6)	Ba _{vi} -O1-Be1-Ba _{ix}	-82.52 (14)
Zn-O1-Be1-O1 ^{xviii}	120.4 (3)	Ba _{vi} -F1-Be1-O1 ^{xviii}	156.20 (10)
Zn-O1-Be-F1	-126.12 (16)	Ba _{ix} -F1-Be1-O1 _{xix}	156.20 (10)

Zn-O1-Be1-Ba ^{vi}	-94.86 (18)	Ba ^x -F1-Be1-O1	156.20 (10)
Zn-O1-Be1-Ba ^{ix}	-177.38 (12)	Ba ^{ix} -F1-Be1-O1 ^{xviii}	36.20 (10)
Zn-O1-Be1-Ba ^x	-89.4 (6)	Ba ^x -F1-Be1-O1 ^{xviii}	-83.80 (10)
B1 ^{vii} -O1-Be1-O1 ^{xviii}	-34.9 (9)	Ba ^x -F1-Be1-O1 ^{xix}	36.20 (10)
B1 ^{vii} -O1-Be1-O1 ^{xix}	-167.9 (4)	Ba ^{ix} -F1-Be1-O1	-83.80 (10)
B1 ^{vii} -O1-Be1-F1	78.6 (5)	Ba ^{vi} -F1-Be1-O1 ^{xix}	-83.80 (10)
B1 ^{vii} -O1-Be1-Ba ^{vi}	109.9 (5)	Ba ^{vi} -F1-Be1-O1	36.20 (10)
B1 ^{vii} -O1-Be1-Ba ^x	115.3 (5)	Ba ^{ix} -F1-Be1-Ba ^{vi}	-120.000 (1)
B1 ^{vii} -O1-Be1-Ba ^{ix}	27.3 (6)	Ba ^{vi} -F1-Be1-Ba ^x	-120.000 (1)
Ba ^{vi} -O1-Be1-O1 ^{xix}	82.2 (4)	Ba ^{vi} -F1-Be1-Ba ^{ix}	120.000 (1)
Ba ^{vi} -O1-Be1-O1 ^{xviii}	-144.8 (4)	Ba ^{ix} -F1-Be1-Ba ^x	120.000 (1)
Ba ^{vi} -O1-Be1-F1	-31.26 (7)	Ba ^x -F1-Be1-Ba ^{vi}	120.000 (1)
Ba ^{vi} -O1-Be1-Ba ^x	5.5 (5)	Ba ^x -F1-Be1-Ba ^{ix}	-120.000 (1)

