# Supporting information

## $SrMBe_2(BO_3)_2F_2$(M=Zn, Mg): Two SBBO-like Compounds Obtained by Cation Regulation

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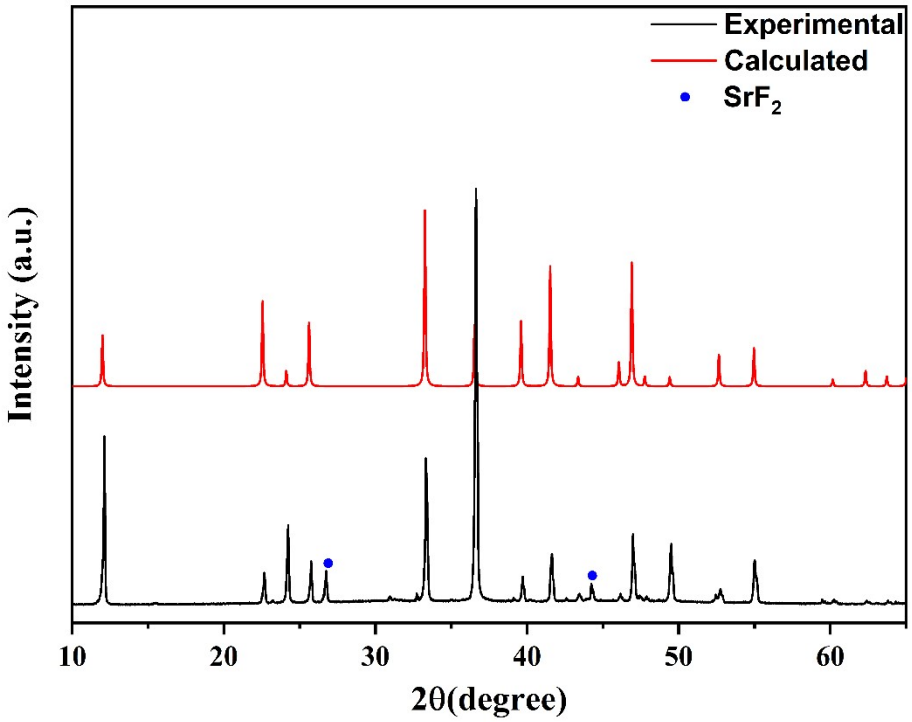


Figure S1. The P-XRD patterns of SMBBF.

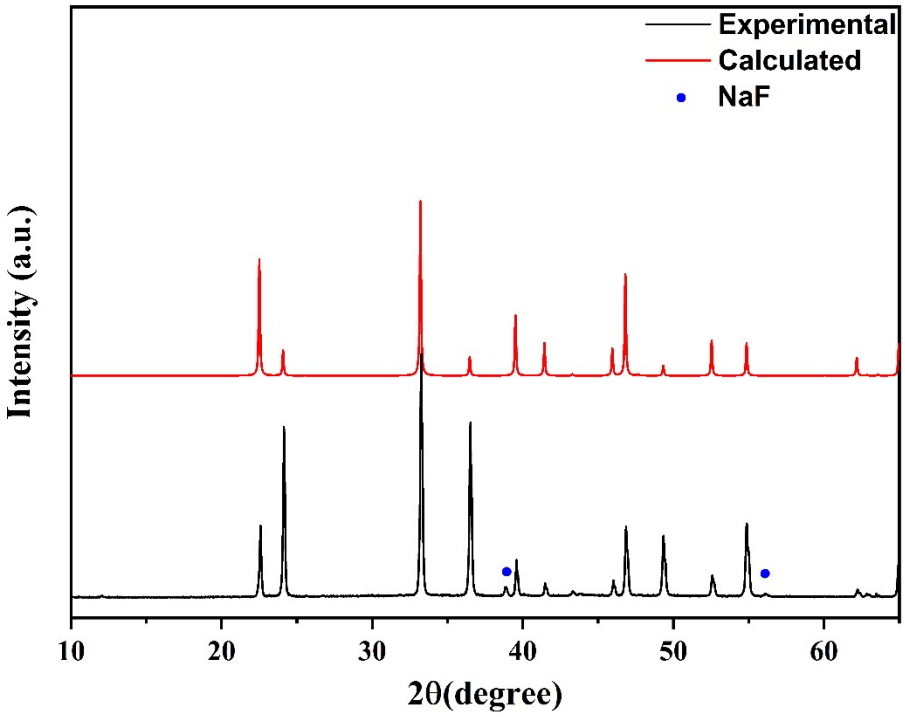


Figure S2. The P-XRD patterns of SZBBF.

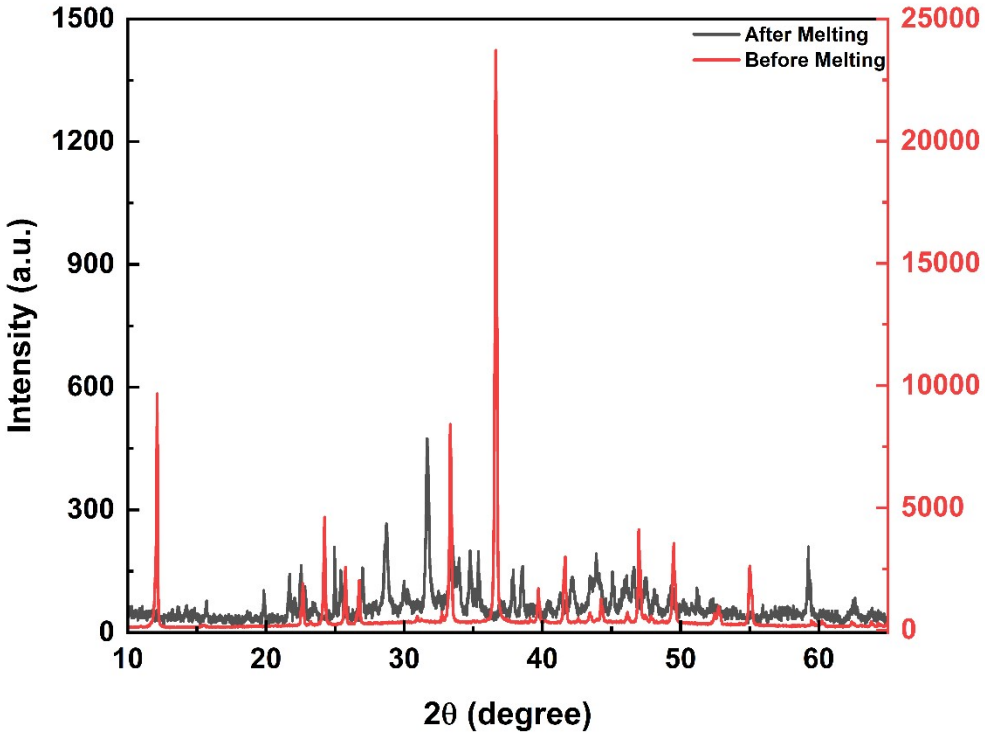


Figure S3. The P-XRD patterns of SMBBF after melting.

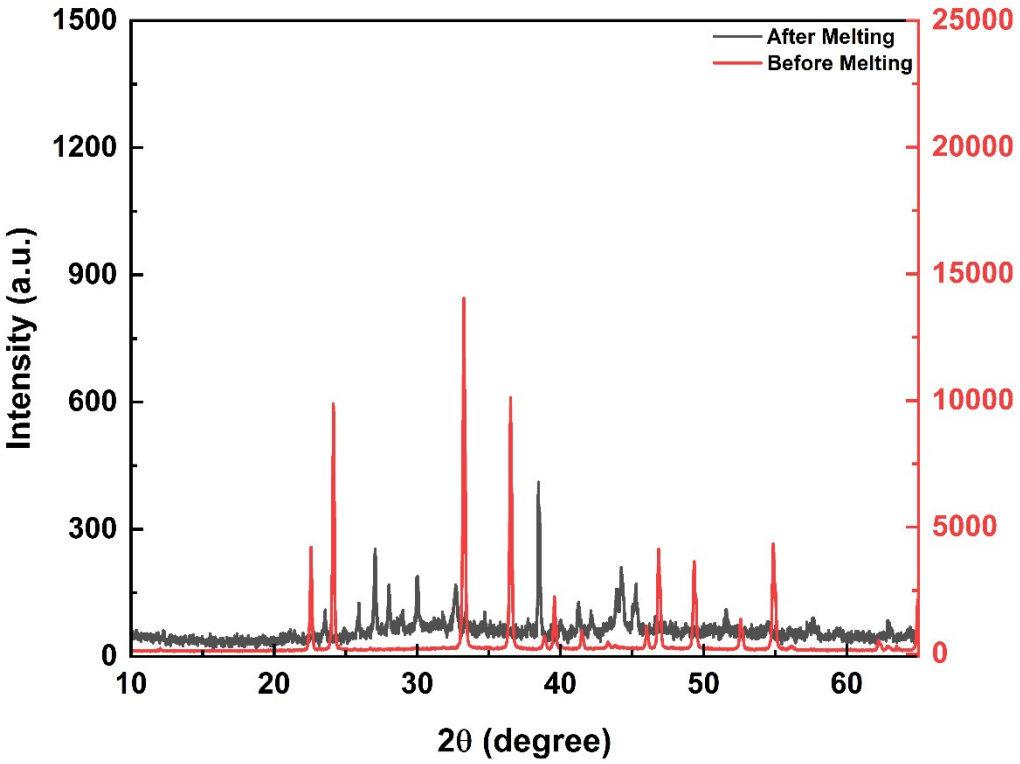


Figure S4. The P-XRD patterns of SZBBF after melting.

**Table S1** Crystal data and structure refinement

| Empirical formula | $SrMgBe_2(BO_3)_2F_2$ | $SrZnBe_2(BO_3)_2F_2$ |
|---|---|---|
| Formula weight | 285.57 | 326.63 |
| Temperature/K | 299.0 | 287.0 |
| Crystal system | trigonal | trigonal |
| Space group | $P\bar{3}$ | $P\bar{3}$ |
| *a*/Å | 4.5482(4) | 4.5577(2) |
| *b*/Å | 4.5482(4) | 4.5577(2) |
| *c*/Å | 7.3726(10) | 7.3840(7) |
| α/° | 90 | 90 |
| β/° | 90 | 90 |
| γ/° | 120 | 120 |
| Volume/Å$^3$ | 132.08(3) | 132.835(17) |
| Z | 1 | 1 |
| $\rho_{calc}$g/cm$^3$ | 3.590 | 4.083 |
| μ/mm$^{-1}$ | 10.360 | 14.589 |
| F(000) | 134.0 | 152.0 |
| Radiation(Å) | Mo Kα(λ= 0.71073) | Mo Kα(λ= 0.71073) |
| Independent reflections | 282 [$R_{int}$ = 0.0621, $R_{sigma}$ = 0.0310] | 281[$R_{int}$=0.0597, $R_{sigma}$=0.0258] |
| Goodness-of-fit on $F^2$ | 1.078 | 1.302 |
| Final R indexes [I>=2σ (I)] | $R_1$=0.0274, $wR_2$=0.0685 | $R_1$=0.0205, $wR_2$=0.0570 |
| Final R indexes [all data] | $R_1$=0.0274, $wR_2$=0.0685 | $R_1$=0.0209, $wR_2$=0.0571 |

**Table S2** Selected bond lengths (Å) and bond angles (deg) for SMBBF and SZBBF.

| SMBBF | | | |
|---|---|---|---|
| bond | length | bond | length |
| Sr1−F3 | 2.6474(4) | B5−O4 | 1.3793(19) |
| Sr1−O4 | 2.8582(19) | F3−Be6 | 1.607(7) |
| Mg2−O4 | 2.0983(18) | O4−Be6 | 1.611(2) |
| angle | degree | angle | degree |
| F3−Sr1−F3 | 180.0 | O4−Mg2−O4 | 96.01(8) |
| F3−Sr1−F3 | 118.41(3) | F3−Be6−O4 | 104.8(2) |
| F3−Sr1−F3 | 61.59(3) | O4−Be5−O4 | 113.75(18) |
| O4−Mg2−O4 | 180.0 | O4−B5−O4 | 119.996(6) |
| O4−Mg2−O4 | 83.99(8) | | |
| SZBBF | | | |
| bond | length | bond | length |
| Sr1−F3 | 2.6531(3) | B5−O4 | 1.3758(11) |
| Sr1−O4 | 2.8578(11) | F3−Be6 | 1.604(5) |
| Zn2−O4 | 2.1148(11) | O4−Be6 | 1.6125(15) |
| angle | degree | angle | degree |
| F3−Sr1−F3 | 180.0 | O4−Zn2−O4 | 96.16(4) |
| F3−Sr1−F3 | 61.607(17) | F3−Be6−O4 | 104.49(15) |
| F3−Sr1−F3 | 118.393(17) | O4−Be5−O4 | 113.96(12) |
| O4−Zn2−O4 | 180.0 | O4−B5−O4 | 120.000(2) |
| O4−Zn2−O4 | 83.84(4) | | |

**Table S3** Atomic coordinates and equivalent isotropic displacement parameters for BMBBF and BCBBF.

| SMBBF | | | | | |
|---|---|---|---|---|---|
| atom | x/a | y/b | z/c | Ueq [Å$^2$ ] | BVS |
| Sr | 1 | 1 | 0.5 | 0.0113(2) | 1.9111 |
| Mg | 0 | 1 | 0 | 0.0075(4) | 2.0081 |
| F | 0.6667 | 1.3333 | 0.4543(4) | 0.0125(6) | 0.9628 |
| O | 0.3431(5) | 0.9747(5) | 0.1807(2) | 0.0086(4) | 1.9857 |
| B | 0.3333 | 0.6667 | 0.1819(7) | 0.0075(8) | 2.9358 |
| Be | 0.6667 | 1.3333 | 0.2363(8) | 0.0071(10) | 2.0244 |
| SZBBF | | | | | |
| atom | x/a | y/b | z/c | Ueq [Å$^2$ ] | BVS |
| Sr | 1 | 0 | 0.5 | 0.0084(2) | 1.8934 |
| Zn | 0 | 0 | 1 | 0.0052(2) | 1.9179 |
| F | 0.6667 | 0.3333 | 0.5459(2) | 0.0098(4) | 0.9573 |
| O | 0.3441(2) | 0.3703(3) | 0.8177.6(16) | 0.0063(3) | 1.9854 |
| B | 0.3333 | 0.6667 | 0.8174(5) | 0.0055(6) | 2.9597 |
| Be | 0.6667 | 0.3333 | 0.7631(6) | 0.0063(6) | 2.0191 |