$BaBi(SeO_3)_2Cl$: a New Polar Material Showing High Second-Harmonic Generation Efficiency Enhanced by Constructive Alignment of Chloride Ions

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Electronic Supplementary Information

Fig. S1. Photo of grown $BaBi(SeO_3)_2Cl$ single crystals with plate-shape.

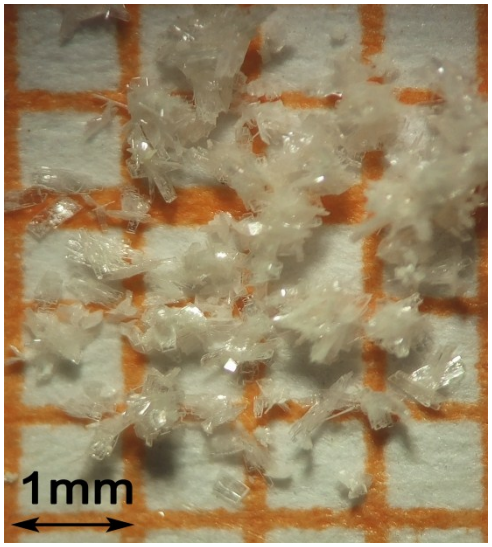

Fig. S2. Comparison of the measured and simulated powder XRD patterns for $BaBi(SeO_3)_2Cl$ (λ = 1.5406 Å). Phase 1: $BaBi(SeO_3)_2Cl$, Phase 2: $Bi_2(SeO_3)_3$.

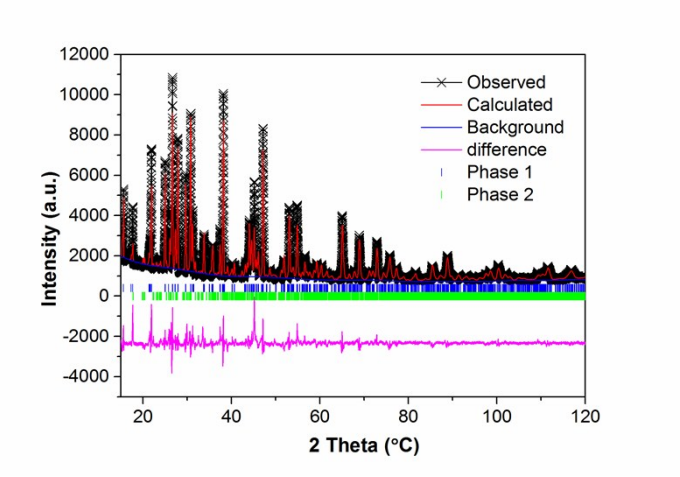

Fig. S3. Calculated SHG coefficients of $BaBi(SeO_3)_2Cl$.

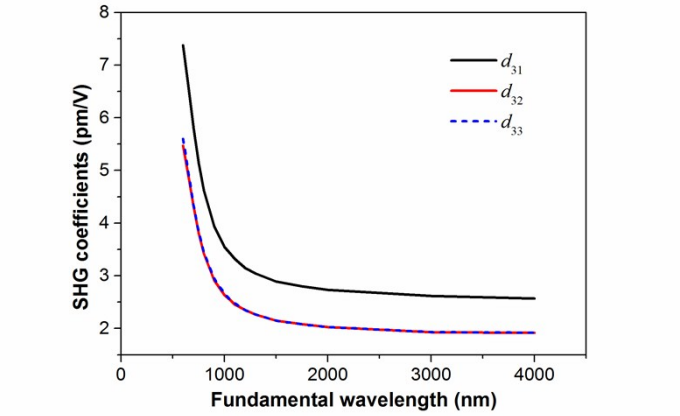

Fig. S4. Calculated refractive index along the principal axis of $BaBi(SeO_3)_2Cl$.

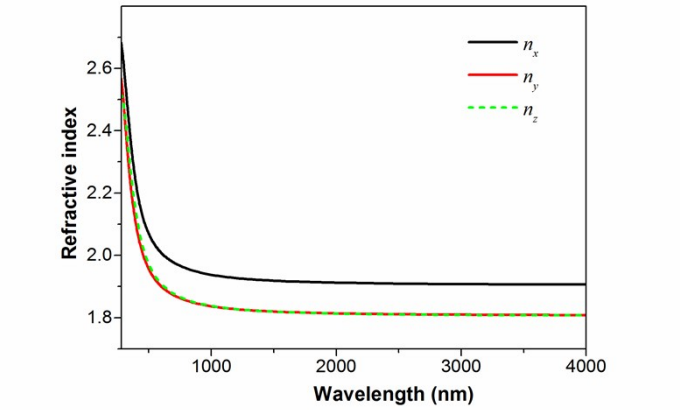

Table S1. The atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for $BaBi(SeO_3)_2Cl$. *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*	*y*	*z*	*U*(eq)

Ba(1)	0	2253(1)	481(1)	10(1)
Bi(1)	0	4245(1)	3378(1)	13(1)
Se(1)	0	308(1)	1893(2)	9(1)
Se(2)	0	1501(1)	5606(2)	7(1)
O(1)	2477(10)	4816(3)	1239(11)	14(1)
O(2)	2507(10)	3368(4)	2170(10)	12(1)
O(3)	0	834(5)	0(15)	14(2)
O(4)	0	2237(4)	4474(14)	10(2)
Cl(1)	0	6469(2)	2417(5)	20(1)

Table S2. The definitions of special *k*-point and corresponding state energies in the first Brilouin zone.

k-point	Lower energy/eV	Higher energy/eV
G (0 0 0)	0	3.610013
Z (0 0 0.5)	–0.20734	3.625932
T (–0.5 0 0.5)	−0.05697	4.212182
Y (–0.5 0 0)	0	4.025642
S (–0.5 0.5 0)	−0.0004	4.032774
X (0 0.5 0)	−0.0668	3.610223
U (0 0.5 0.5)	−0.24126	3.646134
R (–0.5 0.5 0.5)	−0.05678	4.21139