Supporting Information

A new phase-matchable nonlinear optical silicate: $Rb_2ZnSi_3O_8$†

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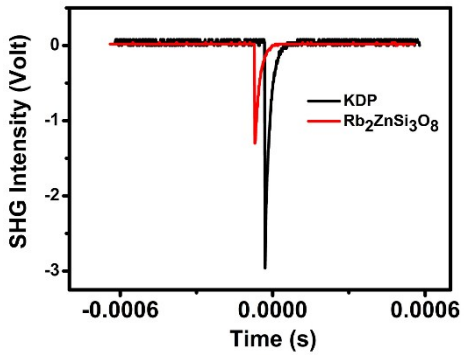


Fig. S1. The SHG response of $Rb_2ZnSi_3O_8$.

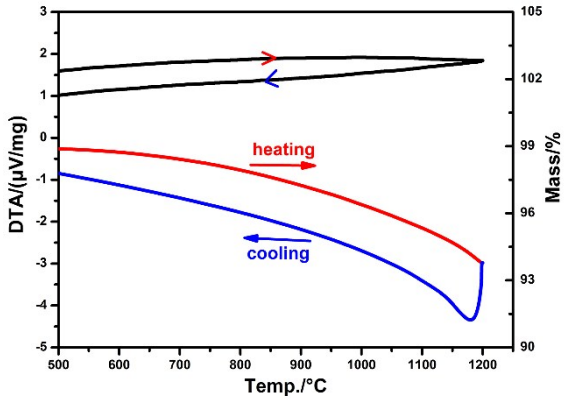
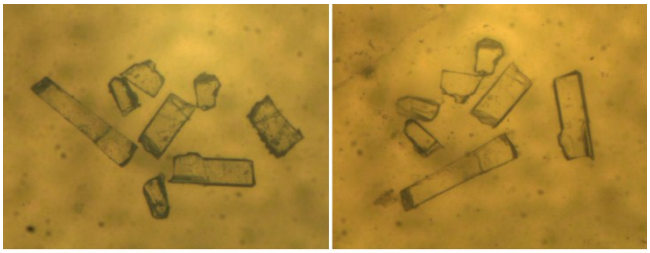


Fig. S2. DTA curves for $Rb_2ZnSi_3O_8$.



(a) **(b)**

Fig. S3 The hygroscopy for $Rb_2ZnSi_3O_8$. (a) Without water at room temperture. (b) Be taken up from the water after 24 h .

Table S1. Calculated nonlinear optical properties of $Rb_2ZnSi_3O_8$.

	d_{14}	d_{16}	d_{22}	d_{23}
$Rb_2ZnSi_3O_8$	-0.053	0.202	-0.357	0.048
Rb	-0.008	0.008	-0.079	0.015
Si-O	-0.021	0.081	-0.314	0.027
Zn-O	-0.035	0.139	-0.240	0.019

Table S2. Atomic coordinates and equivalent isotropic displacement parameters for $Rb_2ZnSi_3O_8$.

Atom	*Wyck.*	*Site*	*S.O.F.*	*x/a*	*y/b*	*z/c*	U_{eq} [Å^2][a]
Rb	4c	1		0.94866(7)	0.5327	0.70962(11)	0.039(1)
Zn2	4c	1	0.5	0.83652(13)	1.0456(4)	0.89779(17)	0.035(1)
Si2	4c	1	0.5	0.83652(13)	1.0456(4)	0.89779(17)	0.035(1)
Si1	4c	1		0.6597(2)	0.5448(6)	0.7168(3)	0.031(1)
O4	4c	1	0.5	0.5009(12)	0.624(2)	0.4490(17)	0.031(1)
O2	4c	1		0.7687(7)	0.7544(14)	0.759(1)	0.044(2)
O3	4c	1		0.6986(9)	0.2729(15)	0.6902(11)	0.051(2)
O1	4c	1	0.5	0.7143(9)	0.536(3)	0.9613(14)	0.032(2)
O5	4c	1	0.5	0.6090(11)	0.548(3)	0.8350(16)	0.034(2)
O6	4c	1	0.5	0.9929(8)	1.135(2)	1.023(2)	0.060(5)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Anisotropic displacement parameters (Å²) for $Rb_2ZnSi_3O_8$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rb1	0.0503(4)	0.0349(4)	0.0462(4)	0.0094(4)	0.0392(3)	0.0096(4)
Zn2	0.0517(6)	0.0252(5)	0.0316(5)	-0.0031(8)	0.0303(5)	-0.0012(6)
Si2	0.0517(6)	0.0252(5)	0.0316(5)	-0.0031(8)	0.0303(5)	-0.0012(6)
Si1	0.0374(8)	0.0242(8)	0.0424(9)	0.0008(11)	0.0318(8)	0.0007(12)
O4	0.034(5)	0.033(5)	0.025(5)	0.000(4)	0.021(5)	0.003(3)
O2	0.035(3)	0.056(4)	0.036(3)	-0.013(3)	0.023(3)	-0.003(3)
O3	0.050(4)	0.046(3)	0.030(3)	0.026(3)	0.019(3)	0.000(3)
O1	0.029(4)	0.039(5)	0.030(4)	-0.006(7)	0.022(4)	0.007(7)
O5	0.040(5)	0.033(5)	0.035(5)	0.009(7)	0.027(4)	0.009(7)
O6	0.104(8)	0.036(5)	0.022(7)	-0.0016(6)	0.037(5)	0.000(4)

Table S4. Selected bond distances (Å) and angles (deg.) for $Rb_2ZnSi_3O_8$.

Rb1—O6 [i]	2.841(13)	Si—O1	1.717(8)
Rb1—O3 [ii]	2.859(7)	Zn2—O6	1.832(10)
Rb1—O4[iii]	2.884(10)	Zn2—O2	1.781(8)
Rb1—O5[iv]	2.995(15)	Zn2—O3[ix]	1.846(7)
Si1—O2	1.617(7)	Si2—O6[viii]	1.542(5)
Si1—O3	1.603(4)	Si2—O1	1.743(8)
O6—Zn2—O1[viii]	116.6(6)	O3[ix]—Zn2—O5[viii]	118.5(5)
O6—Zn2—O2	122.0(5)	O5—Si1—O2	122.1(7)
O1[viii]—Zn2—O2	102.0(5)	O4[xii]—Si1—O3	117.5(5)
O2—Zn2—O3[ix]	103.2(4)	O3—Si1—O1	104.8(6)
O6—Zn2—O3[ix]	111.7(6)	O5—Si1—O4	104.2(5)
O6[v]—Zn2—O5[viii]	102.1(5)	O5—Si1—O3	114.9(8)
O1[viii]—Zn2—O3[ix]	97.9(5)	O4[xii]—Si1—O2	113.5(5)

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