Electronic supplementary information

Single crystal structure and optical properties of nonlinear optical crystal $Rb_{0.94}Ti_{0.94}Ta_{0.06}OPO_4$

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Contents

Fig. S1. (a) UV-vis-NIR and (b) mid-IR transmission spectra of RTP single crystal with the light along a, b and c-directions.

Table S1. Crystal data and structure refinement for $Rb_{0.90}Ti_{0.90}Ta_{0.10}OPO_4$.

Table S2. Selected bond lengths (Å) in $Rb_{0.90}Ti_{0.90}Ta_{0.10}OPO_4$. < Ti(1)-O > represents the mean length of Ti-O bonds.

Table S3. Absorption coeffficients of the $Rb_{0.94}Ti_{0.94}Ta_{0.06}OPO_4$ and RTP crystals.

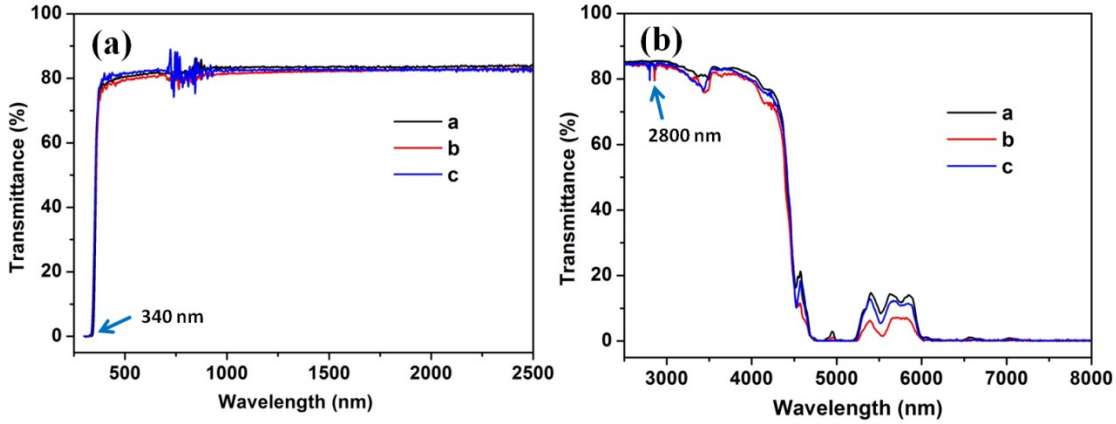

Fig. S1. (a) UV-vis-NIR and (b) mid-IR transmission spectra of RTP single crystal with the light along a, b and c-directions.

Table S1. Crystal data and structure refinement for $Rb_{0.90}Ti_{0.90}Ta_{0.10}OPO_4$.

Empirical formula	$Rb_{0.90}Ti_{0.90}Ta_{0.10}OPO_4$
Formula weight	249.06
Temperature	296(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	a = 12.9584(18) Å, α= 90°.
	b = 6.4968(9) Å, β= 90°
	c = 10.5615(15) Å, γ = 90°
Volume	889.2(2) $Å^3$
Z	8
Density (calculated)	3.721 g/cm^3
Absorption coefficient	34.068mm-1
F(000)	923
Crystal size	0.09 × 0.08 × 0.07 mm3
Theta range for data collection	6.833 ° to 70.265 °
Index ranges	-14 ≤ h ≤ 15, -7 ≤ k ≤ 7, -12 ≤ l ≤12
Independent reflections	1389 [R(int) = 0.0512]
Completeness to theta = 67.679°	98.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1389 / 568 / 148
Goodness-of-fit on F2	1.154
Final R indices [I > 2sigma(I)]	R1 = 0.1180, wR2 = 0.3064
R indices (all data)	R1 = 0.1183, wR2 = 0.3065
Absolute structure parameter	0.75(12)

Table S2. Selected bond lengths (Å) in $Rb_{0.90}Ti_{0.90}Ta_{0.10}OPO_4$. < Ti(1)-O > represents the mean length of Ti-O bonds.

Ti(1)-O_6 octahedron		Ti(2)-O_6 octahedron	
Ti(1)-O(1)	1.96(4)	$Ti(2)^{iii}$-O(3)	2.04(3)
$Ti(1)^{ii}$-O(2)	2.17(4)	$Ti(2)^{ii}$-O(4)	2.05(3)
Ti(1)-O(10)	1.73(4)	$Ti(2)^{iii}$-O(10)	2.05(4)
Ti(1)-O(9)	1.96(4)	Ti(2)-O(9)	1.74(4)
Ti(1)-O(5)	2.03(4)	$Ti(2)^{iii}$-O(7)	2.01(4)
Ti(1)-O(6)	2.10(4)	Ti(2)-O(8)	1.90(4)
< Ti(1)-O >	1.99(6)	< Ti(2)-O >	1.96(9)
P(1)-O_4 tetrahedron		P(2)-O_4 tetrahedron	
P(1)-O(1)	1.52(4)	$P(2)^{v}$ -O(5)	1.52(4)
P(1)-O(2)	1.48(4)	P(2)-O(6)	1.51(4)
P(1)-O(3)	1.56(3)	P(2)-O(7)	1.50(4)
P(1)-O(4)	1.54(3)	$P(2)^{v}$ -O(8)	1.56(4)
< P(1)-O >	1.52(9)	< P(2)-O >	1.52(7)
Rb(1)-O cage		Rb(2)-O cage	
$Rb(1)^{i}$ -O(1)	3.08(4)	Rb(2)-O(1)	2.77(3)
Rb(1)-O(2)	2.77(4)	Rb(2)-O(2)	2.98(4)
$Rb(1)^{iv}$-O(3)	3.00(3)	$Rb(2)^{iv}$-O(4)	2.78(3)
$Rb(1)^{i}$-O(4)	3.11(4)	$Rb(2)^{x}$-O(10)	2.79(4)
$Rb(1)^{vii}$-O(9)	2.84(3)	$Rb(2)^{i}$-O(9)	3.14(3)
$Rb(1)^{vii}$-O(10)	3.10(4)	Rb(2)-O(5)	3.42(3)
$Rb(1)^{i}$-O(6)	2.86(3)	$Rb(2)^{i}$-O(6)	3.04(4)
$Rb(1)^{vii}$-O(7)	3.11(4)	$Rb(2)^{vi}$-O(7)	2.89(3)
$Rb(1)^{viii}$-O(8)	3.07(3)	$Rb(2)^{ix}$-O(8)	3.21(4)
< Rb(1)-O >	2.99(7)	< Rb(2)-O >	3.00(6)
$Ti(1)^{ii}$-Rb(1)	3.701(8)	$Ti(2)^{xi}$-Rb(1)	3.817(1)
$Ti(1)^{ii}$-Rb(2)	3.910(1)	$Ti(2)^{xi}$-Rb(2)	3.671(8)
< Ti(1)-Rb >	3.805(9)	< Ti(2)-Rb >	3.744(4)

Symmetry transformations used to generate equivalent atoms: (i) -x+1,-y+1, z+1/2; (ii) -x+1, -y+1, z-1/2; (iii) -x+1/2, y+1/2, z-1/2; (iv) x, y+1, z; (v) x, y-1, z; (vi) x-1/2, -y+3/2, z; (vii) -x+1/2, y+1/2, z+1/2; (viii) –x+1/2, y-1/2, z+1/2; (ix) -x+1, -y, z+1/2; (x) x-1/2, -y+1/2, z; (xi) -x+1, -y, z-1/2.

Table S3. Absorption coeffficients of the $Rb_{0.94}Ti_{0.94}Ta_{0.06}OPO_4$ and RTP crystals.

	Absorption coeffficient α (cm^{-1}) for RTP		Absorption coeffficient α (cm^{-1}) for RTP:Ta	
Wavelength (nm)	532	1064	532	1064
Light along ***a***-direction	0.42	0.20	0.42	0.19
Light along ***b***-direction	0.48	0.41	0.38	0.15
Light along ***c***-direction	0.08	0.01	0.10	0.06