STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 73 (2017)

Supporting information for article:

The crystal structure of Rb2Ti2O5

Rémi Federicci, Benoit Baptiste, Fabio Finocchi, Florin Popa, Luc Brohan, Keevin Béneut, Paola Giura, Gwenaëlle Rousse, Armel Descamps-Mandine, Thierry Douillard, Abhay Shukla and Brigitte Leridon

Table S1: Anisotropic Displacement Parameters ($^{\circ}$ A$^2\times10^3$) for $Rb_2Ti_2O_5$ at 300 K. The anisotropic displacement factor exponent takes the form: -$2\pi^2(h^2a^{*2}U_{11} + 2hka^*b^*U_{12}+)$.

ATOM	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Rb1	18.9(4)	21.0(4)	24.1(4)	0	6.2(2)	0
Ti1	4.4(5)	10.2(6)	17.3(5)	0	0.7(4)	0
O1	9(3)	13(3)	40(3)	0	9(2)	0
O2	19(2)	22(3)	18.6(19)	0	-1.1(16)	0
O3	5.7(16)	12(2)	24.0(19)	0	-1.7(14)	0

Table S2: Bond Lengths for for $Rb_2Ti_2O_5$ at 300 K.

[1]-X,1-Y,2-Z; [2]-1/2+X,-1/2+Y,+Z; [3]-1/2+X,1/2+Y,+Z; [4]-X,1-Y,1-Z; [5]1/2-X,3/2-Y,2-Z; [6]1/2-X,1/2-Y,2-Z; [7]1/2+X,1/2+Y,+Z; [8]1/2+X,-1/2+Y,+Z; [9]1/2-X,1/2-Y,1-Z; [10]1/2-X,3/2-Y,1-Z; [11]1-X,1-Y,1-Z

ATOM	ATOM	LENGTH(Å)	ATOM	ATOM	LENGTH(Å)
Rb1	Rb1[1]	3.3468(11)	Ti1	O3[9]	1.9861(10)
Rb1	Ti1[2]	3.5945(10)	Ti1	O3	1.988(4)
Rb1	Ti1[3]	3.5945(10)	Ti1	O3[10]	1.9861(10)
Rb1	O3	2.878(4)	Ti1	O1	1.8842(9)
Rb1	O3[4]	3.537(4)	Ti1	O2	1.709(4)
Rb1	O1[2]	3.1400(5)	O3	Rb1[4]	3.537(4)
Rb1	O1[3]	3.1400(5)	O3	Ti1[10]	1.9861(10)
Rb1	O2[2]	3.153(3)	O3	Ti1[9]	1.9861(10)
Rb1	O2[5]	2.894(3)	O1	Rb1[9]	3.1400(5)
Rb1	O2[3]	3.153(3)	O1	Rb1[8]	3.1400(5)
Rb1	O2	3.164(4)	O1	Rb1[10]	3.1400(5)
Rb1	O2[6]	2.894(3)	O1	Rb1[7]	3.1400(5)
Ti1	Rb1[7]	3.5945(10)	O1	Ti[11]	1.8841(9)
Ti1	Rb1[8]	3.5945(10)	O2	RbA[6]	2.894(3)
Ti1	Rb1[9]	3.7281(10)	O2	Rb1[7]	3.153(3)
Ti1	Rb1[10]	3.7281(10)	O2	Rb1[8]	3.153(3)
Ti1	Ti1[10]	3.0920(14)	O2	Rb1[5]	2.894(3)
Ti1	Ti1[9]	3.0920(14)			

Table S3: Anisotropic Displacement Parameters ($^{\circ}$ A$^2\times10^3$) for $Rb_2Ti_2O_5$ at 400 K. The anisotropic displacement factor exponent takes the form: -$2\pi^2(h^2a^{*2}U_{11} + 2hka^*b^*U_{12}+)$.

ATOM	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Rb1	25.2(3)	27.7(3)	28.7(3)	0	8.87(19)	0
Ti1	5.8(3)	12.6(4)	19.2(4)	0	1.6(2)	0
O1	10(2)	19(3)	48(3)	0	15(2)	0
O2	29.5(19)	24(2)	21.9(16)	0	-0.5(14)	0
O3	5.5(12)	13.6(15)	31.8(17)	0	0.2(11)	0

Table S4: Bond Lengths for for $Rb_2Ti_2O_5$ at 400 K.

[1]-X,1-Y,2-Z; [2]-1/2+X,-1/2+Y,+Z; [3]-1/2+X,1/2+Y,+Z; [4]-X,1-Y,1-Z; [5]1/2-X,3/2-Y,2-Z; [6]1/2-X,1/2-Y,2-Z; [7]1/2+X,1/2+Y,+Z; [8]1/2+X,-1/2+Y,+Z; [9]1/2-X,1/2-Y,1-Z; [10]1/2-X,3/2-Y,1-Z; [11]1-X,1-Y,1-Z

ATOM	ATOM	LENGTH(Å)	ATOM	ATOM	LENGTH(Å)
Rb1	Rb1[1]	3.3518(10)	Ti1	O3[9]	1.9824(9)
Rb1	Ti1[2]	3.6000(9)	Ti1	O3	1.992(3)
Rb1	Ti1[3]	3.6000(9)	Ti1	O3[10]	1.9824(9)
Rb1	O3	2.893(4)	Ti1	O1	1.8844(8)
Rb1	O3[4]	3.542(3)	Ti1	O2	1.705(4)
Rb1	O1[3]	3.1464(5)	O3	Rb1[4]	3.542(3)
Rb1	O1[2]	3.1464(5)	O3	Ti1[10]	1.9824(9)
Rb1	O2[2]	3.154(3)	O3	Ti1[9]	1.9824(9)
Rb1	O2	3.164(4)	O1	Rb1[7]	3.1464(5)
Rb1	O2[5]	2.899(3)	O1	Rb1[10]	3.1464(5)
Rb1	O2[3]	3.154(3)	O1	Rb1[8]	3.1464(5)
Rb1	O2[6]	2.899(3)	O1	Rb1[9]	3.1464(5)
Ti1	Rb1[7]	3.6000(9)	O1	Ti[11]	1.8844(7)
Ti1	Rb1[8]	3.6000(9)	O2	Rb1[6]	2.899(3)
Ti1	Rb1[9]	3.7338(9)	O2	Rb1[8]	3.154(3)
Ti1	Rb1[10]	3.7338(9)	O2	Rb1[5]	2.899(3)
Ti1	Rb1[10]	3.0926(12)	O2	Rb1[7]	3.154(3)
Ti1	Rb1[9]	3.0926(12)			

Table S5: Anisotropic Displacement Parameters ($^{\circ}A^2 \times 10^3$) for $Rb_2Ti_2O_5$ at 150 K. The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + 2hka^*b^*U_{12}+)$.

ATOM	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Rb1	12.3(6)	17.9(7)	13.1(6)	0	-1.6(4)	0
Ti1	5.5(9)	10.9(10)	10.5(9)	0	-4.3(6)	0
O1	4(4)	19(5)	22(5)	0	0(4)	0
O2	13(3)	15(3)	16(3)	0	-4(3)	0
O3	6(3)	16(4)	19(3)	0	-6(3)	0

Table S6: Bond Lengths for for $Rb_2Ti_2O_5$ at 150 K.

[1]-X,1-Y,2-Z; [2]-1/2+X,-1/2+Y,+Z; [3]-1/2+X,1/2+Y,+Z; [4]-X,1-Y,1-Z; [5]1/2-X,3/2-Y,2-Z; [6]1/2-X,1/2-Y,2-Z; [7]1/2+X,1/2+Y,+Z; [8]1/2+X,-1/2+Y,+Z; [9]1/2-X,1/2-Y,1-Z; [10]1/2-X,3/2-Y,1-Z; [11]1-X,1-Y,1-Z

ATOM	ATOM	LENGTH(Å)	ATOM	ATOM	LENGTH(Å)
Rb1	Rb1[1]	3.3460(16)	Ti1	O3	1.8910(15)
Rb1	Ti1[2]	3.5845(17)	Ti1	O3[8]	1.9805(17)
Rb1	Ti1[3]	3.5845(17)	Ti1	O3	2.000(6)
Rb1	O1[2]	3.1265(7)	Ti1	O3[9]	1.9805(17)
Rb1	O1[3]	3.1265(7)	Ti1	O2	1.710(7)
Rb1	O3[4]	3.513(6)	O1	Rb1[7]	3.1266(7)
Rb1	O3	2.877(7)	O1	Rb1[8]	3.1266(7)
Rb1	O2	3.171(6)	O1	Rb1[9]	3.1266(7)
Rb1	O2[2]	3.148(5)	O1	Rb1[10]	3.1266(7)
Rb1	O2[5]	2.878(5)	O1	Ti1[11]	1.8910(15)
Rb1	O2[6]	2.878(5)	O3	Rb1[4]	3.513(6)
Rb1	O2[3]	3.148(5)	O3	Ti[10]	1.9805(17)
Ti1	Rb1[7]	3.5845(17)	O3	Ti1[8]	1.9805(17)
Ti1	Rb1[8]	3.7221(16)	O2	Rb1[5]	2.878(5)
Ti1	Rb1[9]	3.7221(16)	O2	Rb1[7]	3.148(5)
Ti1	Rb1[10]	3.5845(17)	O2	Rb1[10]	3.148(5)
Ti1	Ti1[9]	3.091(2)	O2	Rb1[6]	2.878(5)
Ti1	Ti1[8]	3.091(2)			

2. Additional XRD powder diffractograms

In Fig.1 are represented the X-Ray Diffractograms at 400 K and 200 K for a powder sample of $Rb_2Ti_2O_5$. Similar diffractograms at 300 K and 100 K are also presented in the text. All diffractograms are identical, ruling out strong evidence for a structural phase transition in temperature.

3. Representations of the DFT phonon modes calculated with GGA functional

Table S7: List of vibrational phonon modes calculated with the Density Functional Theory using Generalized Gradient Approximation for the $Rb_2Ti_2O_5$ system. High Raman intensity range : [1500 - 15000], medium Raman intensity range : [150 - 1500], low Raman intensity range : [0 - 150]. The phonon mode representations are displayed in figure 2, 3, 4, 5, 6, 7, 8

N°	ν (cm^{-1})	RAMAN INTENSITY (au)	N°	ν (cm^{-1})	RAMAN INTENSITY (au)
1	0	low	28	240	high
2	0	low	29	252	medium
3	0	low	30	254	high
4	0	low	31	256	low
5	0	low	32	282	medium
6	0	low	33	292	low
7	9	low	34	301	high
8	63	low	35	309	low
9	67	low	36	319	high
10	73	low	37	387	low
11	86	low	38	400	low
12	87	low	39	413	low
13	88	low	40	432	low
14	89	low	41	444	medium
15	92	low	42	447	high
16	115	low	43	457	low
17	125	low	44	498	low
18	134	medium	45	507	high
19	145	low	46	594	high
20	155	low	47	599	medium
21	165	medium	48	624	low
22	183	low	49	721	low
23	193	low	50	759	low
24	219	high	51	759	low
25	225	medium	52	846	low
26	230	medium	53	879	medium
27	234	medium	54	881	high

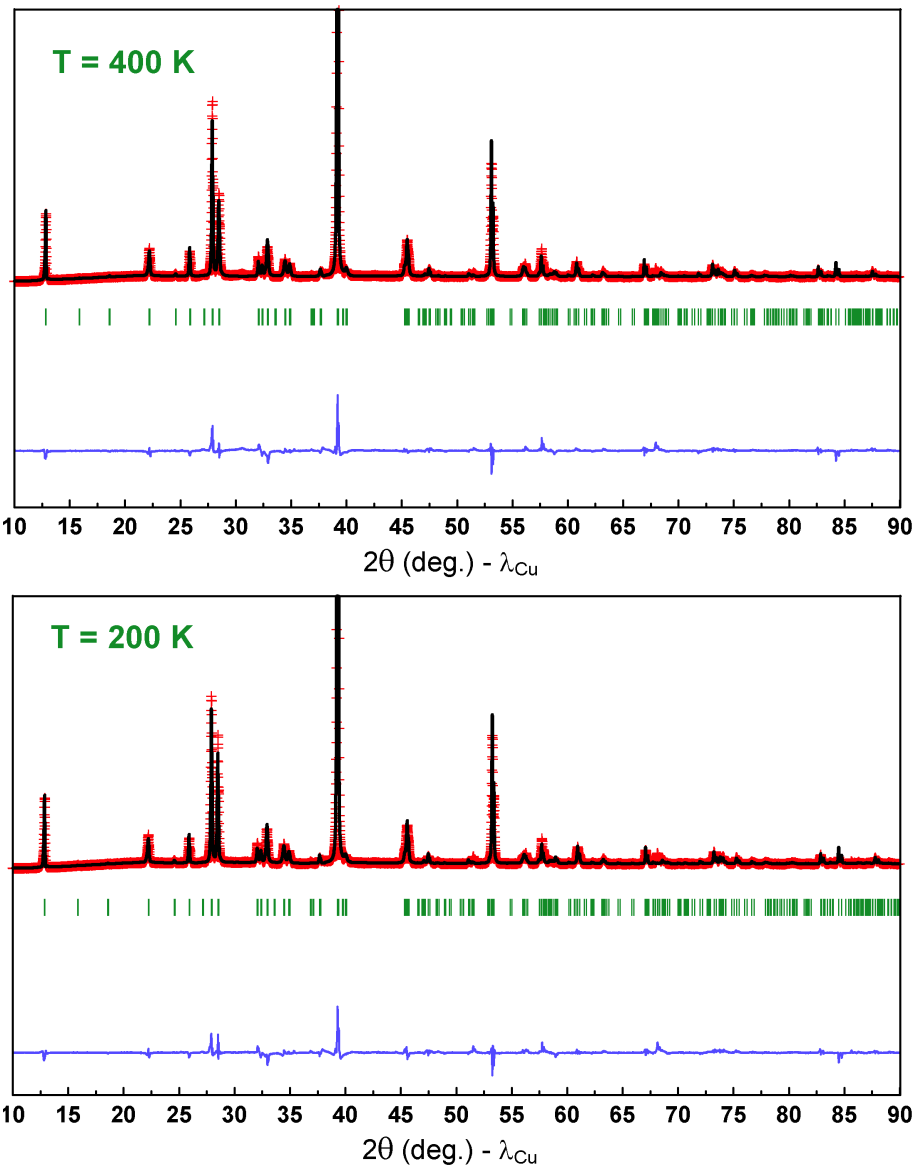

Figure S1: Rietveld refinements and powder X-Ray diffraction patterns (λ Cu) for $Rb_2Ti_2O_5$ at 400 K (top) and 200 K (bottom). The red circles are the experimental points, the black line is the calculated pattern, the green vertical ticks refer to Bragg reflections and the blue line is the difference between observed and calculated patterns. Similar diffractograms at 300 K and 100 K are presented in the text.

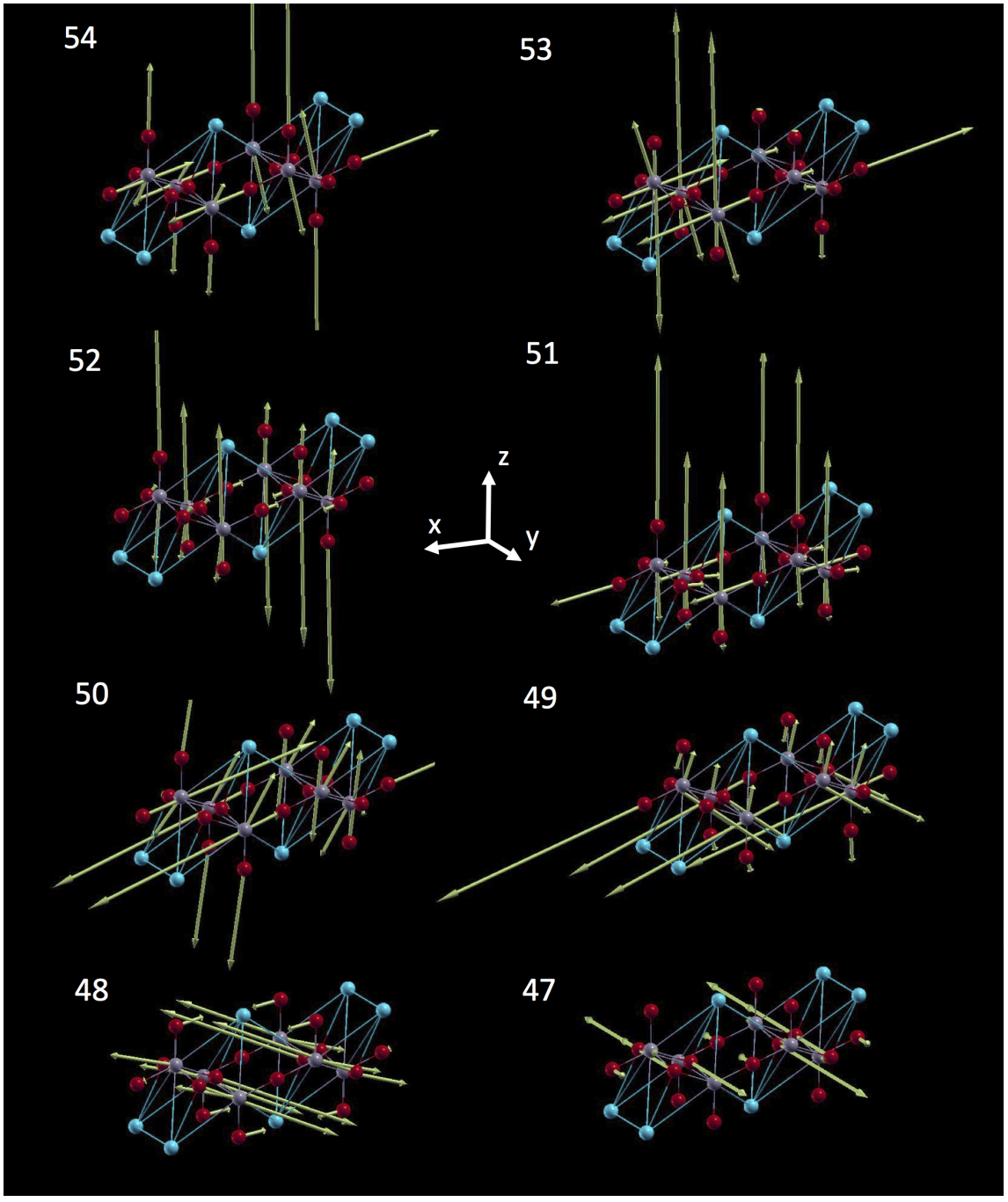

Figure S2: Representations of the vibrational phonon modes N° 54, 53, 52, 51, 50, 49, 48 and 47 calculated using Density Function Theory for $Rb_2Ti_2O_5$ system. The frequency and Raman intensity of the related phonon modes are displayed in Table 7.

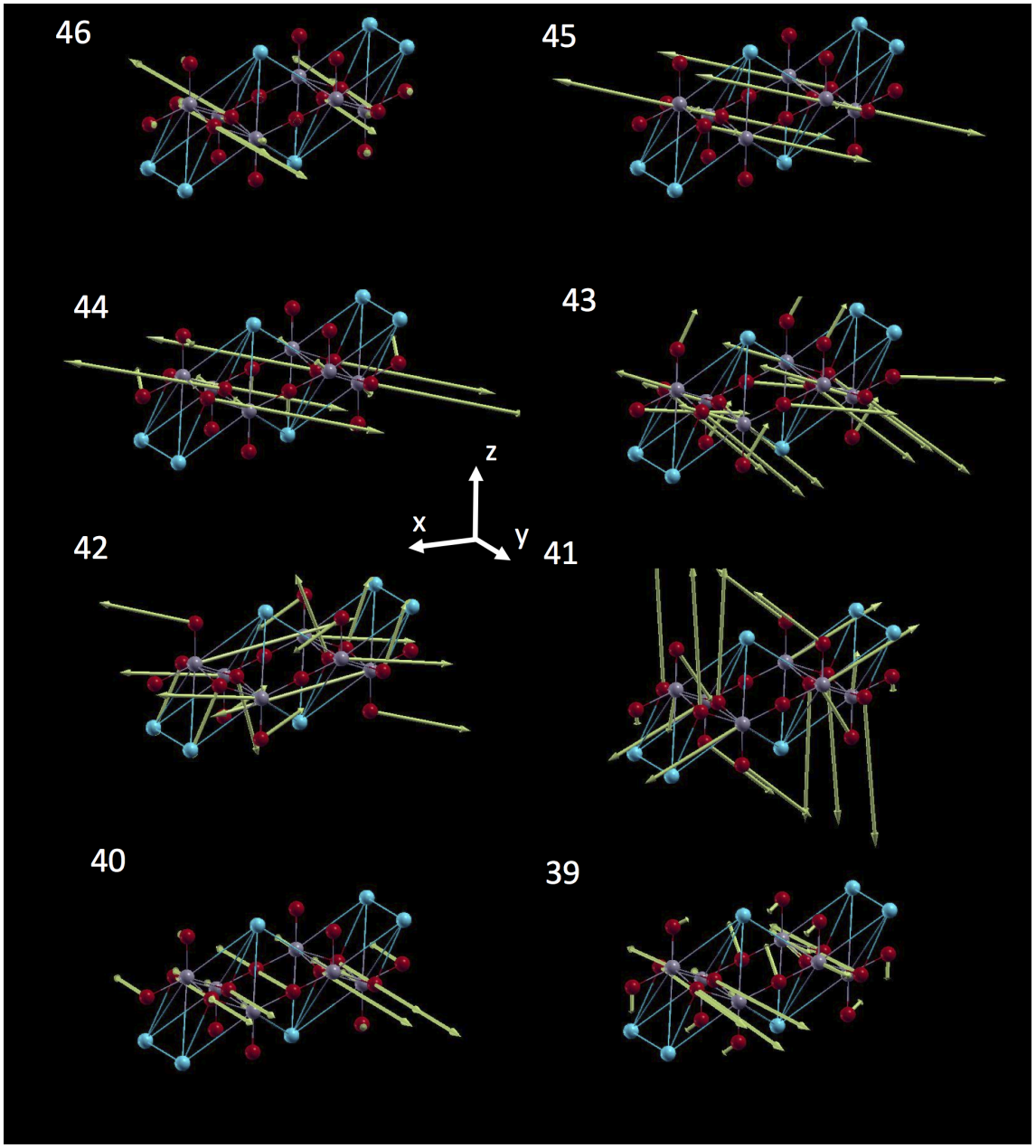

Figure S3: Representations of the vibrational phonon modes N° 46, 45, 44, 43, 42, 41, 40 and 39 calculated using Density Function Theory for $Rb_2Ti_2O_5$ system. The frequency and Raman intensity of the related phonon modes are displayed in Table 7.

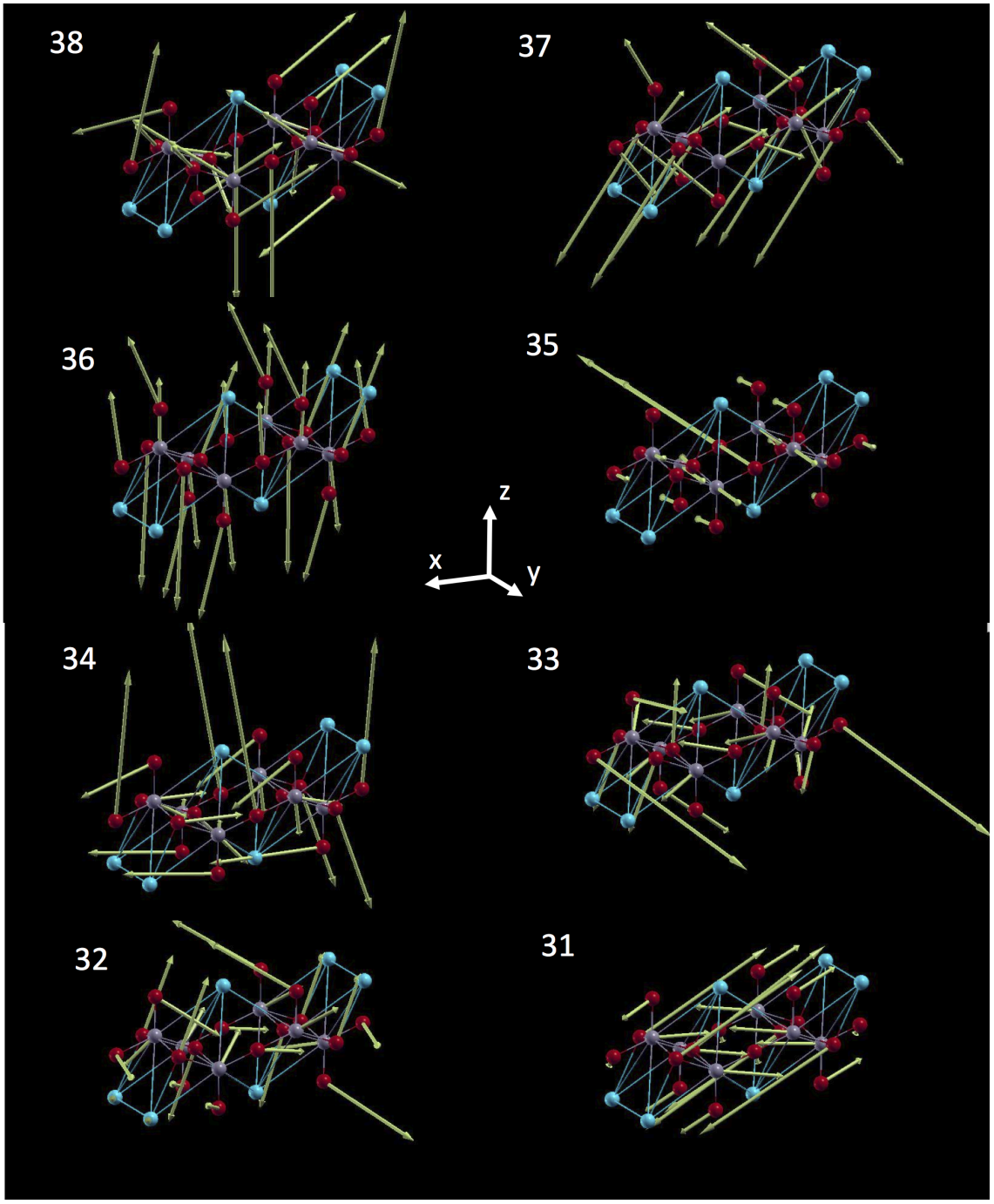

Figure S4: Representations of the vibrational phonon modes N° 38, 37, 36, 35, 34, 33, 32 and 31 calculated using Density Function Theory for $Rb_2Ti_2O_5$ system. The frequency and Raman intensity of the related phonon modes are displayed in Table 7.

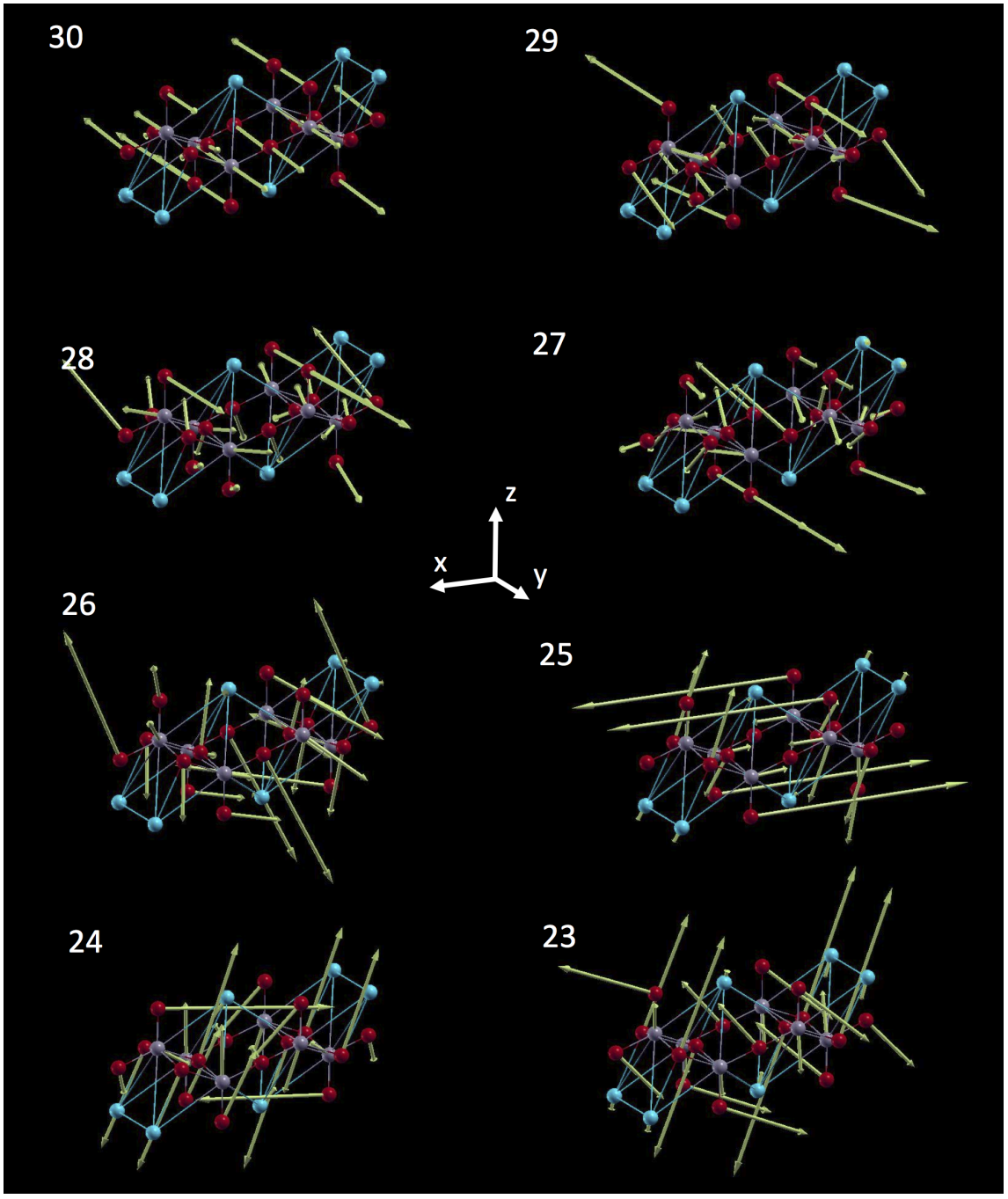

Figure S5: Representations of the vibrational phonon modes N° 30, 29, 28, 27, 26, 25, 24 and 23 calculated using Density Function Theory for $Rb_2Ti_2O_5$ system. The frequency and Raman intensity of the related phonon modes are displayed in Table 7.

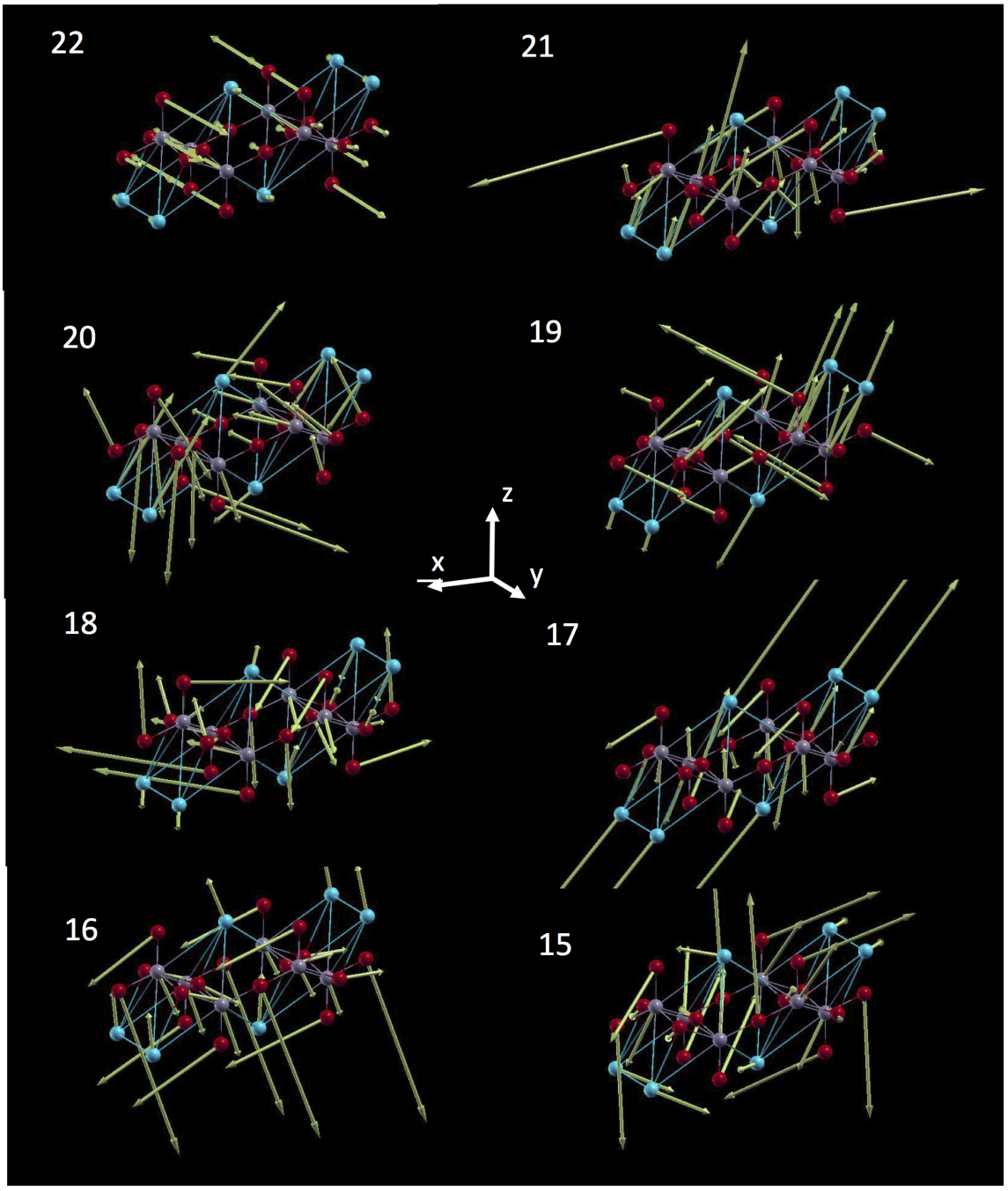

Figure S6: Representations of the vibrational phonon modes N° 22, 21, 20, 19, 18, 17, 16 and 15 calculated using Density Function Theory for $Rb_2Ti_2O_5$ system. The frequency and Raman intensity of the related phonon modes are displayed in Table 7.

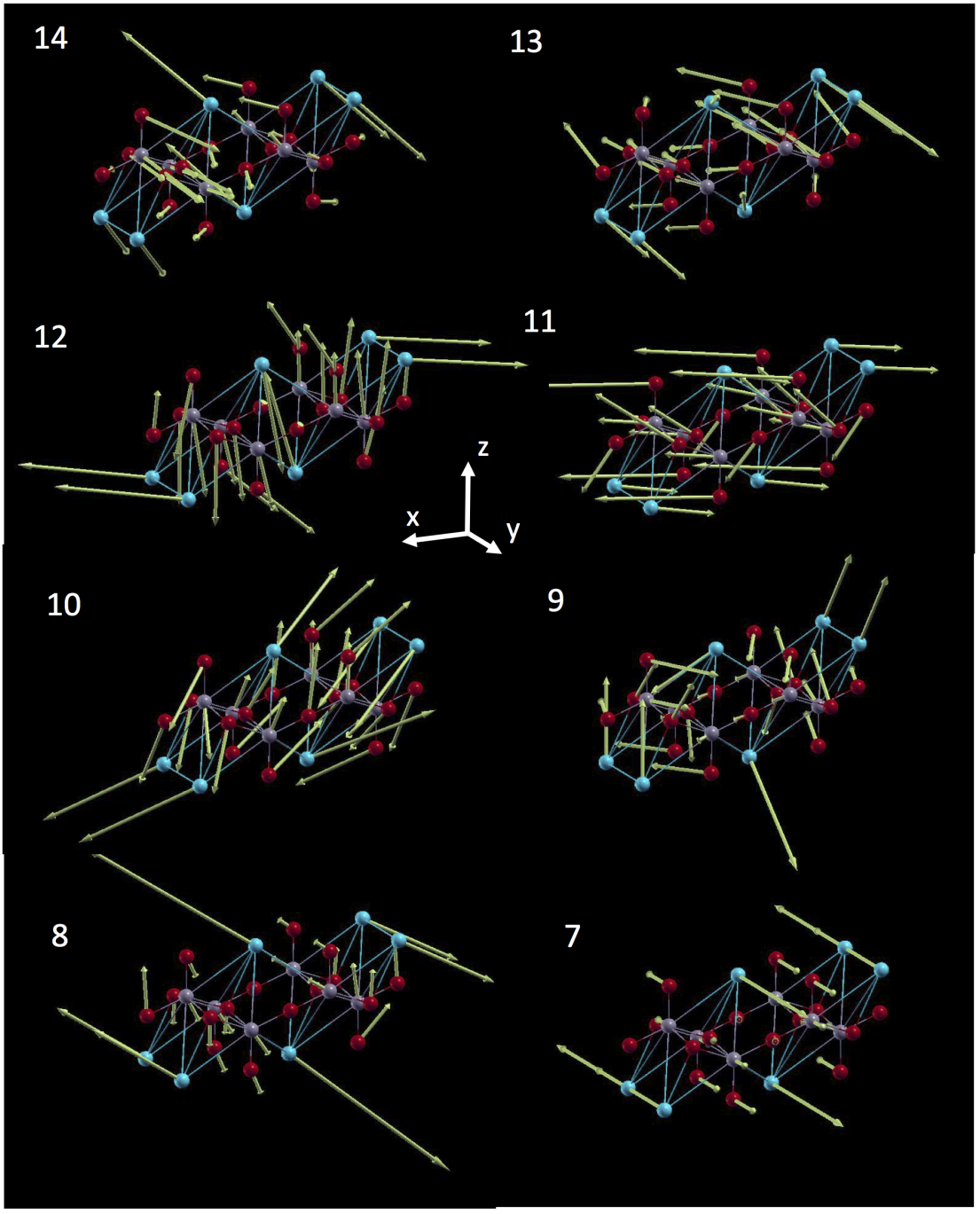

Figure S7: Representations of the vibrational phonon modes N° 14, 13, 12, 11, 10, 9, 8 and 7 calculated using Density Function Theory for $Rb_2Ti_2O_5$ system. The frequency and Raman intensity of the related phonon modes are displayed in Table 7.

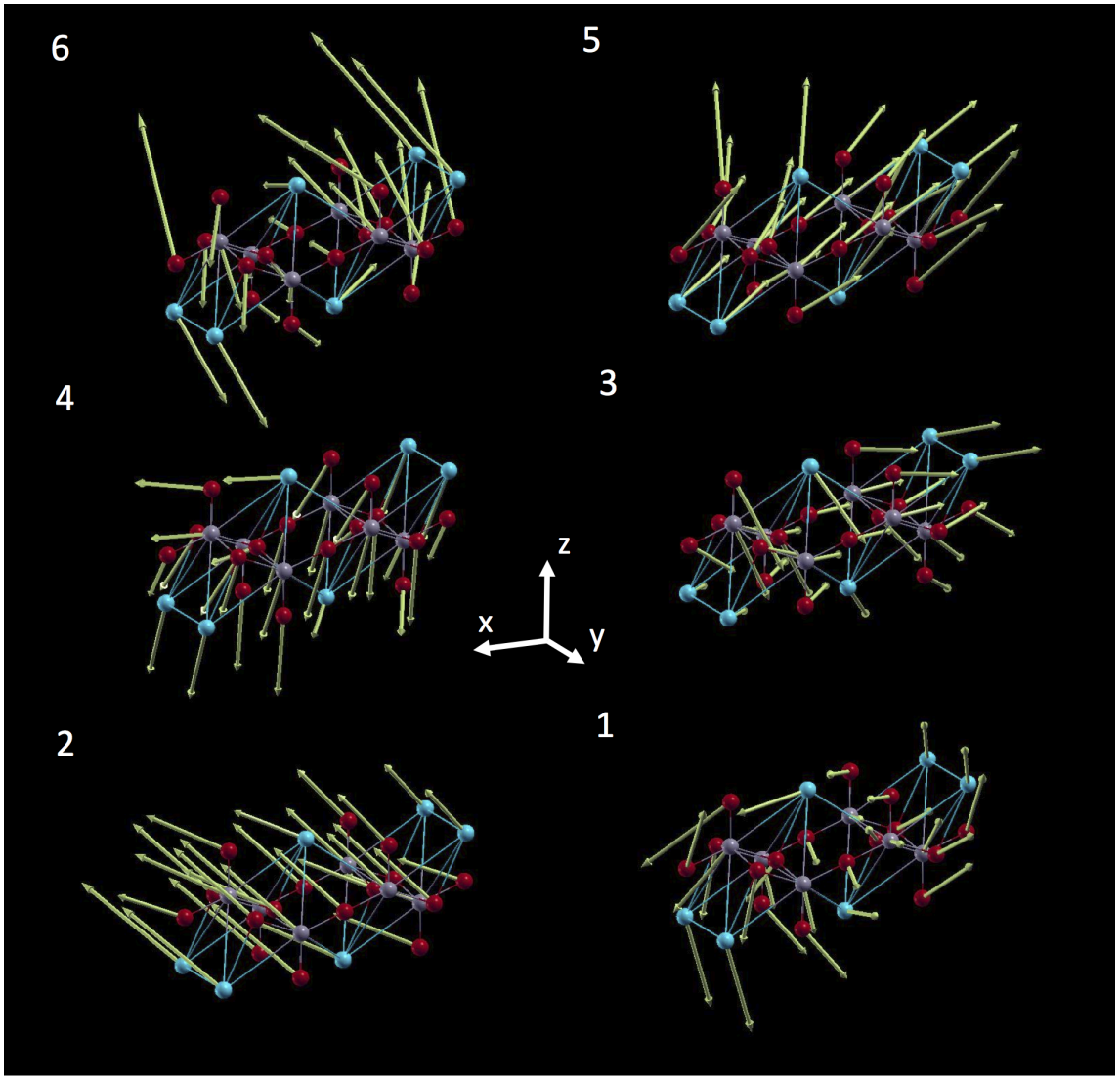

Figure S8: Representations of the vibrational phonon modes N° 6, 5, 4, 3, 2 and 1 calculated using Density Function Theory for $Rb_2Ti_2O_5$ system. The frequency and Raman intensity of the related phonon modes are displayed in Table 7.