Electronic Supplementary Information (ESI)

$Rb_8Nb_{10}Ge_6O_{41}$: A new niobium-germanate crystal featuring unique one-dimensional $[Nb_7O_{30}]_\infty$ chains and wide mid-IR transparency

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1. **Table S1.** The final atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å2 \times 10^3$) for $Rb_8Nb_{10}Ge_6O_{41}$, U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor, and the BVS for each atom in asymmetric unit.

2. **Table S1.** Selected bond lengths (Å) and angles (deg.) for $Rb_8Nb_{10}Ge_6O_{41}$.

3. **Fig. S1**. EDS observations of $Rb_8Nb_{10}Ge_6O_{41}$. (a) Surface morphology of $Rb_8Nb_{10}Ge_6O_{41}$. (b) atomic ratio of various elements. (c-f) Rb, Nb, Ge, and O mapping results, respectively.

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Atom	x	y	z	U(eq)	BVS
Nb(1)	5322(2)	6681(1)	3654(1)	26(1)	5.22
Rb(1)	10125(2)	8338(1)	3485(1)	40(1)	0.94
Ge(1)	0	3571(2)	2500	19(1)	4.08
O(1)	7345(14)	7090(8)	4129(4)	37(3)	2.03
Nb(2)	5000	5000	5000	41(1)	5.38
Ge(2)	2124(2)	5758(1)	2559(1)	22(1)	4.32
Rb(2)	-156(3)	4944(2)	4074(1)	57(1)	0.85
O(2)	3680(13)	7545(8)	4138(4)	35(3)	1.98
Nb(3)	2916(2)	7656(1)	4989(1)	34(1)	5.12
O(3)	4846(16)	5444(9)	4144(4)	49(3)	1.94
O(4)	3190(17)	6440(9)	3111(4)	54(3)	1.97
O(5)	6500(20)	3830(10)	4765(5)	45(4)	1.69
O(6)	2708(17)	4148(9)	4889(4)	56(3)	1.87
O(7)	585(16)	7008(10)	4818(5)	56(3)	1.93
O(8)	3151(19)	5678(9)	1875(4)	62(4)	2.00
O(9)	0	6382(14)	2500	98(9)	1.78
O(10)	1664(12)	4439(8)	2831(4)	28(2)	2.03
O(11)	1040(12)	2908(7)	1920(4)	27(2)	2.13

Table S2. Selected bond lengths (Å) and angles (deg.) for $Rb_8Nb_{10}Ge_6O_{41}$

Nb(1)-O(1)	1.878(10)	Ge(2)-O(10)	1.782(9)
Nb(1)-O(3)	1.916(10)	Rb(2)-O(6)	2.927(11)
Nb(1)-O(2)	1.931(10)	Rb(2)-O(7)	3.101(12)
Nb(1)-O(4)	1.984(11)	Rb(2)-O(10)	3.122(9)
Nb(1)-O(8)#1	2.041(10)	Rb(2)-O(8)#9	3.162(12)
Nb(1)-O(11)#2	2.057(9)	Rb(2)-O(6)#11	3.164(13)
Rb(1)-O(1)	2.921(10)	Rb(2)-O(2)#12	3.174(11)
Rb(1)-O(3)#7	3.003(11)	Rb(2)-O(5)#6	3.187(14)
Rb(1)-O(10)#7	3.068(9)	Rb(2)-O(11)#9	3.421(9)
Rb(1)-O(2)#3	3.119(9)	Rb(2)-O(7)#11	3.471(12)
Rb(1)-O(5)#7	3.137(14)	O(2)-Nb(3)	1.973(9)
Rb(1)-O(11)#2	3.144(9)	Nb(3)-O(7)	1.912(12)
Rb(1)-O(9)#3	3.273(13)	Nb(3)-O(6)#4	1.925(11)
Rb(1)-O(8)#2	3.343(12)	Nb(3)-O(5)#10	1.974(13)
Rb(1)-O(4)#3	3.349(13)	Nb(3)-O(7)#8	2.028(12)
Rb(1)-O(7)#3	3.407(12)	O(1)-Nb(1)-O(3)	92.3(4)
Rb(1)-O(6)#7	3.634(12)	O(1)-Nb(1)-O(2)	91.1(4)
Ge(1)-O(11)#9	1.705(9)	O(3)-Nb(1)-O(2)	91.2(4)
Ge(1)-O(11)	1.705(9)	O(1)-Nb(1)-O(4)	172.6(4)
Ge(1)-O(10)	1.779(9)	O(3)-Nb(1)-O(4)	94.7(4)
Ge(1)-O(10)#9	1.779(9)	O(2)-Nb(1)-O(4)	86.6(5)
O(1)-Nb(3)#8	2.026(9)	O(1)-Nb(1)-O(8)#1	93.7(5)
O(1)-Rb(2)#3	3.232(10)	O(3)-Nb(1)-O(8)#1	86.2(4)
Nb(2)-O(5)	1.893(14)	O(2)-Nb(1)-O(8)#1	174.6(5)
Nb(2)-O(5)#10	1.893(14)	O(4)-Nb(1)-O(8)#1	88.9(5)
Nb(2)-O(3)	1.982(10)	O(1)-Nb(1)-O(11)#2	87.1(4)
Nb(2)-O(3)#10	1.982(10)	O(3)-Nb(1)-O(11)#2	173.8(4)
Nb(2)-O(6)#10	1.988(11)	O(2)-Nb(1)-O(11)#2	95.0(4)
Nb(2)-O(6)	1.988(11)	O(4)-Nb(1)-O(11)#2	86.2(4)
Ge(2)-O(4)	1.680(10)	O(8)#1-Nb(1)-O(11)#2	87.7(4)
Ge(2)-O(8)	1.694(10)	O(1)-Rb(1)-O(3)#7	103.3(3)
Ge(2)-O(9)	1.731(8)	O(1)-Rb(1)-O(10)#7	173.7(3)

O(3)#7-Rb(1)-O(10)#7	80.5(3)	O(1)-Rb(1)-O(7)#3	52.0(3)
O(1)-Rb(1)-O(2)#3	100.1(3)	O(3)#7-Rb(1)-O(7)#3	90.0(3)
O(3)#7-Rb(1)-O(2)#3	92.5(3)	O(10)#7-Rb(1)-O(7)#3	123.6(3)
O(10)#7-Rb(1)-O(2)#3	74.5(2)	O(2)#3-Rb(1)-O(7)#3	50.3(3)
O(1)-Rb(1)-O(5)#7	53.1(3)	O(5)#7-Rb(1)-O(7)#3	49.1(3)
O(3)#7-Rb(1)-O(5)#7	52.5(3)	O(11)#2-Rb(1)-O(7)#3	105.0(3)
O(10)#7-Rb(1)-O(5)#7	128.8(3)	O(9)#3-Rb(1)-O(7)#3	102.8(3)
O(2)#3-Rb(1)-O(5)#7	87.2(3)	O(8)#2-Rb(1)-O(7)#3	132.3(3)
O(1)-Rb(1)-O(11)#2	53.0(2)	O(4)#3-Rb(1)-O(7)#3	78.9(3)
O(3)#7-Rb(1)-O(11)#2	107.1(3)	O(1)-Rb(1)-O(6)#7	91.5(3)
O(10)#7-Rb(1)-O(11)#2	131.1(2)	O(3)#7-Rb(1)-O(6)#7	48.4(3)
O(2)#3-Rb(1)-O(11)#2	149.2(3)	O(10)#7-Rb(1)-O(6)#7	87.3(3)
O(5)#7-Rb(1)-O(11)#2	86.4(3)	O(2)#3-Rb(1)-O(6)#7	48.0(2)
O(1)-Rb(1)-O(9)#3	85.0(2)	O(5)#7-Rb(1)-O(6)#7	48.1(3)
O(3)#7-Rb(1)-O(9)#3	167.2(3)	O(11)#2-Rb(1)-O(6)#7	134.5(2)
O(10)#7-Rb(1)-O(9)#3	92.2(2)	O(9)#3-Rb(1)-O(6)#7	142.3(2)
O(2)#3-Rb(1)-O(9)#3	95.6(2)	O(8)#2-Rb(1)-O(6)#7	98.5(2)
O(5)#7-Rb(1)-O(9)#3	137.7(3)	O(4)#3-Rb(1)-O(6)#7	96.9(2)
O(11)#2-Rb(1)-O(9)#3	69.90(17)	O(7)#3-Rb(1)-O(6)#7	49.3(3)
O(1)#7-Rb(1)-O(8)#2	106.5(3)	O(11)#9-Ge(1)-O(11)	122.1(6)
O(3)#7-Rb(1)-O(8)#2	50.1(3)	O(11)#9-Ge(1)-O(10)	106.4(4)
O(10)#7-Rb(1)-O(8)#2	79.8(3)	O(11)-Ge(1)-O(10)	107.8(4)
O(2)#3-Rb(1)-O(8)#2	137.8(3)	O(11)#9-Ge(1)-O(10)#9	107.8(4)
O(5)#7-Rb(1)-O(8)#2	83.4(3)	O(11)-Ge(1)-O(10)#9	106.4(4)
O(11)#2-Rb(1)-O(8)#2	71.1(3)	O(10)-Ge(1)-O(10)#9	105.2(6)
O(9)#3-Rb(1)-O(8)#2	118.5(2)	O(5)-Nb(2)-O(5)#10	180.0
O(1)-Rb(1)-O(4)#3	101.8(3)	O(5)-Nb(2)-O(3)	89.0(5)
O(3)#7-Rb(1)-O(4)#3	137.0(3)	O(5)#10-Nb(2)-O(3)	91.0(5)
O(10)#7-Rb(1)-O(4)#3	72.2(2)	O(5)-Nb(2)-O(3)#10	91.0(5)
O(2)#3-Rb(1)-O(4)#3	48.9(3)	O(5)#10-Nb(2)-O(3)#10	89.0(5)
O(5)#7-Rb(1)-O(4)#3	127.7(3)	O(3)-Nb(2)-O(3)#10	180.0(7)
O(11)#2-Rb(1)-O(4)#3	115.8(3)	O(5)-Nb(2)-O(6)#10	87.9(6)
O(9)#3-Rb(1)-O(4)#3	47.8(2)	O(5)#10-Nb(2)-O(6)#10	92.1(6)
O(8)#2-Rb(1)-O(4)#3	147.2(3)	O(3)-Nb(2)-O(6)#10	91.0(4)

O(3)#10-Nb(2)-O(6)#10	89.0(4)	O(7)-Rb(2)-O(1)#6	52.6(3)
O(5)-Nb(2)-O(6)	92.1(6)	O(10)-Rb(2)-O(1)#6	115.9(2)
O(5)#10-Nb(2)-O(6)	87.9(6)	O(8)#9-Rb(2)-O(1)#6	53.2(2)
O(3)-Nb(2)-O(6)	89.0(4)	O(6)#11-Rb(2)-O(1)#6	49.3(3)
O(3)#10-Nb(2)-O(6)	91.0(4)	O(2)#12-Rb(2)-O(1)#6	164.8(3)
O(6)#10-Nb(2)-O(6)	180.0	O(5)#6-Rb(2)-O(1)#6	85.1(3)
O(4)-Ge(2)-O(8)	118.8(6)	O(6)-Rb(2)-O(11)#9	106.3(3)
O(4)-Ge(2)-O(9)	103.8(6)	O(7)-Rb(2)-O(11)#9	171.7(3)
O(8)-Ge(2)-O(9)	110.5(5)	O(10)-Rb(2)-O(11)#9	50.2(2)
O(4)-Ge(2)-O(10)	107.6(4)	O(8)#9-Rb(2)-O(11)#9	69.8(2)
O(8)-Ge(2)-O(10)	109.4(5)	O(6)#11-Rb(2)-O(11)#9	128.6(3)
O(9)-Ge(2)-O(10)	105.8(6)	O(2)#12-Rb(2)-O(11)#9	52.8(2)
O(6)-Rb(2)-O(7)	80.1(3)	O(5)#6-Rb(2)-O(11)#9	81.1(3)
O(6)-Rb(2)-O(10)	100.2(3)	O(1)#6-Rb(2)-O(11)#9	122.1(2)
O(7)-Rb(2)-O(10)	124.3(3)	O(6)-Rb(2)-O(7)#11	52.4(3)
O(6)-Rb(2)-O(8)#9	175.8(3)	O(7)-Rb(2)-O(7)#11	102.6(3)
O(7)-Rb(2)-O(8)#9	103.5(3)	O(10)-Rb(2)-O(7)#11	121.6(3)
O(10)-Rb(2)-O(8)#9	76.1(2)	O(8)#9-Rb(2)-O(7)#11	127.8(3)
O(6)-Rb(2)-O(6)#11	95.0(3)	O(6)#11-Rb(2)-O(7)#11	71.4(3)
O(7)-Rb(2)-O(6)#11	54.4(3)	O(2)#12-Rb(2)-O(7)#11	48.8(3)
O(10)-Rb(2)-O(6)#11	164.2(3)	O(5)#6-Rb(2)-O(7)#11	44.5(3)
O(8)#9-Rb(2)-O(6)#11	88.8(3)	O(1)#6-Rb(2)-O(7)#11	120.1(3)
O(6)-Rb(2)-O(2)#12	54.2(3)	O(11)#9-Rb(2)-O(7)#11	85.6(2)
O(7)-Rb(2)-O(2)#12	134.2(3)	O(7)-Nb(3)-O(6)#4	100.2(6)
O(10)-Rb(2)-O(2)#12	73.0(2)	O(7)-Nb(3)-O(2)	91.7(4)
O(8)#9-Rb(2)-O(2)#12	122.3(3)	O(6)#4-Nb(3)-O(2)	91.3(4)
O(6)#11-Rb(2)-O(2)#12	120.1(3)	O(7)-Nb(3)-O(5)#10	81.3(6)
O(6)-Rb(2)-O(5)#6	95.5(3)	O(6)#4-Nb(3)-O(5)#10	170.5(4)
O(7)-Rb(2)-O(5)#6	103.7(3)	O(2)-Nb(3)-O(5)#10	98.1(5)
O(10)-Rb(2)-O(5)#6	131.3(3)	O(7)-Nb(3)-O(1)#14	94.4(4)
O(8)#9-Rb(2)-O(5)#6	85.6(3)	O(6)#4-Nb(3)-O(1)#14	85.0(4)
O(6)#11-Rb(2)-O(5)#6	50.2(3)	O(2)-Nb(3)-O(1)#14	173.4(4)
O(2)#12-Rb(2)-O(5)#6	80.0(3)	O(5)#10-Nb(3)-O(1)#14	85.5(5)
O(6)-Rb(2)-O(1)#6	130.9(3)	O(7)-Nb(3)-O(7)#8	167.0(2)

O(6)#4-Nb(3)-O(7)#8	92.9(5)	O(5)#10-Nb(3)-O(7)#8	86.0(6)
O(2)-Nb(3)-O(7)#8	87.1(4)	O(1)#14-Nb(3)-O(7)#8	87.6(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2 #2 x+1/2,y+1/2,-z+1/2 #3 x+1,y,z

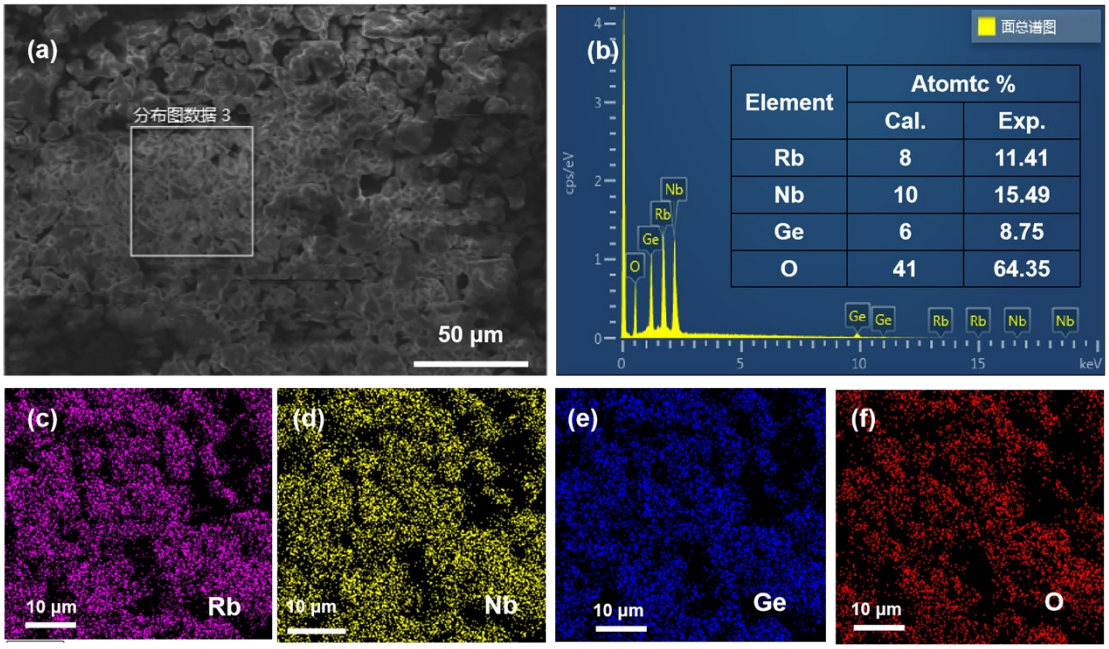
#4 -x+1/2,y+1/2,z #5 -x+3/2,y-1/2,z #6 x-1,y,z

#7 -x+3/2,y+1/2,z #8 x+1/2,-y+3/2,-z+1 #9 -x,y,-z+1/2

#10 -x+1,-y+1,-z+1 #11 -x,-y+1,-z+1 #12 -x+1/2,y-1/2,z

#13 x-3/2,y-1/2,-z+1/2 #14 x-1/2,-y+3/2,-z+1

#15 x-1/2,y-1/2,-z+1/2



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