Supplementary Information

$KRb_2(NO_3)_2Cl$: a New Birefringent Crystal Exhibiting Perovskite-Related Framework and Short Cutoff Edge

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Table S1. Crystal data and structure refinement for $KRb_2(NO_3)_2Cl$.

Empirical formula	$KRb_2(NO_3)_2Cl$
Formula weight	369.51
Temperature	273.15 K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	*Pbam*
Unit cell dimensions	a = 12.1863(6) Å b = 12.4072(7) Å c = 5.8203(3) Å
Volume	880.02(8) $Å^3$
Z	4
Density (calculated)	2.789 Mg/m^3
Absorption coefficient	11.892 mm^{-1}
F(000)	688
Crystal size	0.17 × 0.16 × 0.15 mm^3
Theta range for data collection	2.343 to 27.492°
Index ranges	-14≤h≤15, -15≤k≤16, -7≤l≤7
Reflections collected	6869
Independent reflections	1092 [R_{int} = 0.0544]
Completeness to theta = 27.4920°	98.2 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1092 / 0 / 68
Goodness-of-fit on F^2	1.111
Final R indices [$F_o^2>2\sigma(F_c^2)$][a]	R_1 = 0.0277, wR_2 = 0.0691
R indices (all data)[a]	R_1 = 0.0323, wR_2 = 0.0719
Largest diff. peak and hole	0.843 and -0.426 e.$Å^{-3}$

[a] $R_1=\sum||F_o|-|F_c||/\sum|F_o|$ and $wR_2=[\sum w(F_o^2-F_c^2)^2/\sum w F_o^4]^{1/2}$ for $F_o^2>2\sigma(F_o^2)$

Table S2. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2×10^3) for $KRb_2(NO_3)_2Cl$.

Atom	x	y	z	U(eq)
K(1)	2682(1)	1927(1)	5000	27(1)
Rb(1)	1629(1)	4778(1)	0	27(1)
Rb(2)	4904(1)	3363(1)	0	30(1)
N(1)	3784(3)	4629(3)	5000	24(1)
N(2)	5313(4)	1216(3)	5000	29(1)
O(1)	3591(2)	5096(2)	3139(5)	38(1)
O(2)	4160(3)	3697(3)	5000	39(1)
O(3)	4804(2)	1278(2)	6870(5)	39(1)
O(4)	6329(3)	1074(4)	5000	48(1)
Cl(1)	2458(1)	2329(1)	0	24 (1)

Table S3. Bond lengths [Å] and angles [°] for $KRb_2(NO_3)_2Cl$.

Rb(1)-Cl(1)	3.2020(13)	O(4)#6-Rb(1)-O(4)#7	137.96(18)
Rb(1)-Cl(1)#1	3.3551(13)	Cl(1)#8-Rb(2)-Cl(1)	141.310(18)
Rb(1)-O(1)	3.035(3)	Cl(1)#8-Rb(2)-O(1)#2	130.68(5)
Rb(1)-O(1)#2	3.035(3)	Cl(1)#8-Rb(2)-O(1)	130.68(5)
Rb(1)-O(3)#3	3.159(3)	O(1)#9-Rb(2)-Cl(1)	139.31(5)
Rb(1)-O(3)#4	3.136(3)	O(1)#2-Rb(2)-Cl(1)	78.98(5)
Rb(1)-O(3)#5	3.136(3)	O(1)#9-Rb(2)-Cl(1)#8	66.95(5)
Rb(1)-O(3)#6	3.159(3)	O(1)-Rb(2)-Cl(1)	78.98(6)
Rb(1)-O(4)#6	3.1176(18)	O(1)#10-Rb(2)-Cl(1)	139.31(5)
Rb(1)-O(4)#7	3.1176(18)	O(1)#10-Rb(2)-Cl(1)#8	66.95(5)
Rb(2)-Cl(1)	3.2460(12)	O(1)#9-Rb(2)-O(1)#2	101.94(7)
Rb(2)-Cl(1)#8	3.2275(12)	O(1)#10-Rb(2)-O(1)	101.94(7)
Rb(2)-O(1)#9	3.218(3)	O(1)#9-Rb(2)-O(1)	64.38(9)
Rb(2)-O(1)#2	3.244(3)	O(1)#10-Rb(2)-O(1)#2	64.38(9)
Rb(2)-O(1)	3.244(3)	O(1)-Rb(2)-O(1)#2	68.53(9)
Rb(2)-O(1)#10	3.218(3)	O(1)#9-Rb(2)-O(1)#10	69.17(10)
Rb(2)-O(3)#11	3.166(3)	O(3)#12-Rb(2)-Cl(1)	69.01(5)
Rb(2)-O(3)#12	3.166(3)	O(3)#11-Rb(2)-Cl(1)#8	79.63(5)
Rb(2)-O(2)	3.0763(13)	O(3)#11-Rb(2)-Cl(1)	69.01(5)
Rb(2)-O(2)#12	3.0764(13)	O(3)#12-Rb(2)-Cl(1)#8	79.63(5)
K(1)-Cl(1)#13	2.9653(3)	O(3)#11-Rb(2)-O(1)	101.45(7)
K(1)-Cl(1)	2.9653(3)	O(3)#11-Rb(2)-O(1)#2	147.85(7)
K(1)-O(1)#14	2.956(3)	O(3)#12-Rb(2)-O(1)#10	100.40(7)
K(1)-O(1)#15	2.956(3)	O(3)#12-Rb(2)-O(1)#2	101.45(7)
K(1)-O(3)	2.918(3)	O(3)#11-Rb(2)-O(1)#9	100.40(7)
K(1)-O(3)#11	2.918(3)	O(3)#11-Rb(2)-O(1)#10	146.51(8)
K(1)-O(2)	2.841(4)	O(3)#12-Rb(2)-O(1)	147.85(7)
K(1)-O(4)#7	2.979(5)	O(3)#12-Rb(2)-O(1)#9	146.51(8)
N(1)-O(1)	1.251(3)	O(3)#12-Rb(2)-O(3)#11	70.27(10)
N(1)-O(2)	1.251(3)	O(2)#12-Rb(2)-Cl(1)#8	108.67(7)
N(1)-O(1)#11	1.243(5)	O(2)#12-Rb(2)-Cl(1)	77.44(8)
N(2)-O(4)	1.250(6)	O(2)-Rb(2)-Cl(1)	77.44(8)
N(2)-O(3)	1.255(3)	O(2)-Rb(2)-Cl(1)#8	108.67(7)
N(2)-O(3)#11	1.255(3)	O(2)-Rb(2)-O(1)#9	63.31(9)
		O(2)#12-Rb(2)-O(1)#2	39.87(8)
Cl(1)-Rb(1)-Cl(1)#1	142.235(17)	O(2)#12-Rb(2)-O(1)#9	128.67(9)
O(1)#2-Rb(1)-Cl(1)	82.83(6)	O(2)-Rb(2)-O(1)#10	128.67(9)

O(1)#2-Rb(1)-Cl(1)#1	67.40(5)	O(2)#12-Rb(2)-O(1)#10	63.31(9)
O(1)-Rb(1)-Cl(1)	82.83(6)	O(2)-Rb(2)-O(1)#2	107.32(8)
O(1)-Rb(1)-Cl(1)#1	67.40(5)	O(2)-Rb(2)-O(1)	39.86(8)
O(1)#2-Rb(1)-O(1)	74.02(11)	O(2)#12-Rb(2)-O(1)	107.32(8)
O(1)#2-Rb(1)-O(3)#4	135.32(7)	O(2)-Rb(2)-O(3)#12	130.04(9)
O(1)#2-Rb(1)-O(3)#6	105.15(8)	O(2)#12-Rb(2)-O(3)#11	130.04(9)
O(1)-Rb(1)-O(3)#6	162.88(8)	O(2)#12-Rb(2)-O(3)#12	63.54(9)
O(1)#2-Rb(1)-O(3)#5	90.67(8)	O(2)-Rb(2)-O(3)#11	63.54(9)
O(1)-Rb(1)-O(3)#5	135.32(7)	O(2)-Rb(2)-O(2)#12	142.16(14)
O(1)#2-Rb(1)-O(3)#3	162.88(8)	Cl(1)#13-K(1)-Cl(1)	157.87(6)
O(1)-Rb(1)-O(3)#3	105.15(8)	Cl(1)#13-K(1)-O(4)#7	78.97(3)
O(1)-Rb(1)-O(3)#4	90.67(8)	Cl(1)-K(1)-O(4)#7	78.97(3)
O(1)-Rb(1)-O(4)#6	134.30(9)	O(1)#14-K(1)-Rb(1)#14	48.49(6)
O(1)#2-Rb(1)-O(4)#6	64.83(9)	O(1)#15-K(1)-Rb(1)#14	82.30(6)
O(1)#2-Rb(1)-O(4)#7	134.30(9)	O(1)#14-K(1)-Rb(1)#16	82.30(6)
O(1)-Rb(1)-O(4)#7	64.83(9)	O(1)#15-K(1)-Rb(1)#16	48.49(6)
O(3)#4-Rb(1)-Cl(1)	137.64(5)	O(1)#14-K(1)-Cl(1)	116.13(6)
O(3)#6-Rb(1)-Cl(1)#1	128.66(6)	O(1)#15-K(1)-Cl(1)	73.80(6)
O(3)#3-Rb(1)-Cl(1)	80.12(6)	O(1)#14-K(1)-Cl(1)#13	73.80(6)
O(3)#5-Rb(1)-Cl(1)	137.64(5)	O(1)#15-K(1)-Cl(1)#13	116.13(6)
O(3)#3-Rb(1)-Cl(1)#1	128.66(6)	O(1)#15-K(1)-O(1)#14	43.00(10)
O(3)#4-Rb(1)-Cl(1)#1	67.96(5)	O(1)#15-K(1)-O(4)#7	110.43(10)
O(3)#6-Rb(1)-Cl(1)	80.12(6)	K(1)#8-O(4)-Rb(1)#17	102.56(8)
O(3)#5-Rb(1)-Cl(1)#1	67.96(5)	K(1)#8-O(4)-Rb(1)#8	102.56(8)
O(3)#4-Rb(1)-O(3)#3	61.26(10)	N(2)#11-O(4)-Rb(1)#17	99.42(12)
O(3)#4-Rb(1)-O(3)#5	71.04(11)	N(2)-O(4)-Rb(1)#17	99.42(12)
O(4)#7-Rb(1)-O(3)#4	66.02(10)	N(2)-O(4)-Rb(1)#8	99.42(12)
O(4)#7-Rb(1)-O(3)#6	108.38(9)	N(2)#11-O(4)-Rb(1)#8	99.42(12)
O(4)#6-Rb(1)-O(3)#5	66.02(10)	N(2)#11-O(4)-K(1)#8	115.5(4)
O(4)#6-Rb(1)-O(3)#4	132.71(9)	N(2)-O(4)-K(1)#8	115.5(4)

Symmetry transformations used to generate equivalent atoms:

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

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

#6 x-1/2,-y+1/2,z-1 #7 x-1/2,-y+1/2,z

#8 x+1/2,-y+1/2,z #9 -x+1,-y+1,z #10 -x+1,-y+1,-z

#11 x,y,-z+1 #12 x,y,z-1 #13 x,y,z+1

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

#16 -x+1/2,y-1/2,-z #17 x+1/2,-y+1/2,z+1

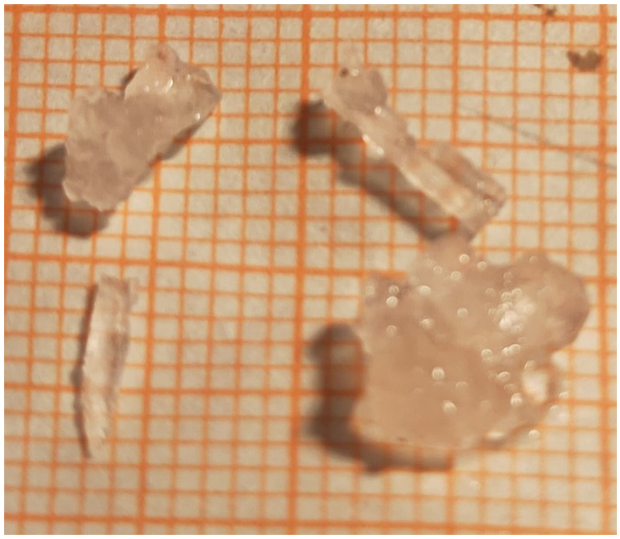

Figure S1. The photograph of the $KRb_2(NO_3)_2Cl$ crystal plate (the minimum scale is 1 mm).

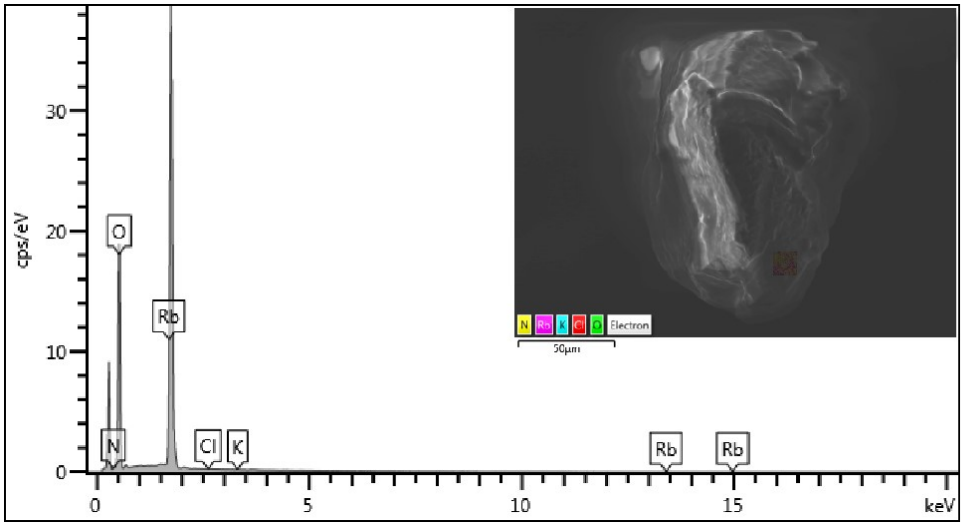

Figure S2. EDS spectrum of $KRb_2(NO_3)_2Cl$.

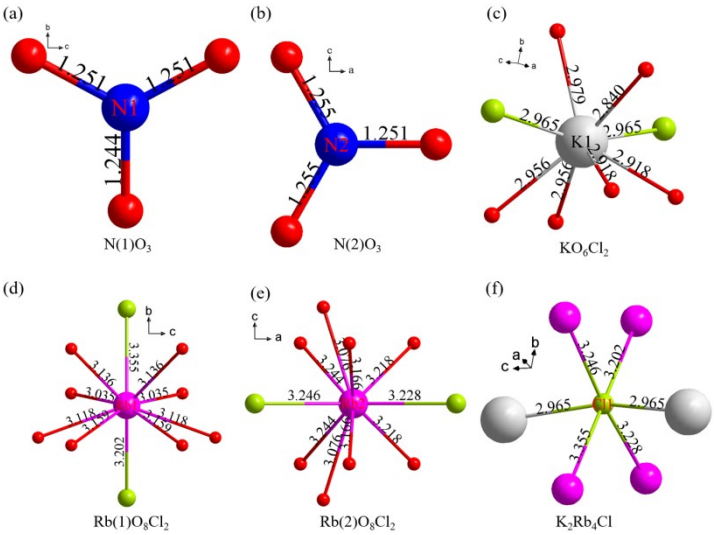

Figure S3. (a) the $N(1)O_3$ triangle; (b) the $N(2)O_3$ triangle; (c) the KO_6F_2 polyhedra; (d) the $Rb(1)O_8Cl_2$ polyhedra ; (e) the $Rb(2)O_8Cl_2$ polyhedra; (f) the ClK_2R_4 octahedra.

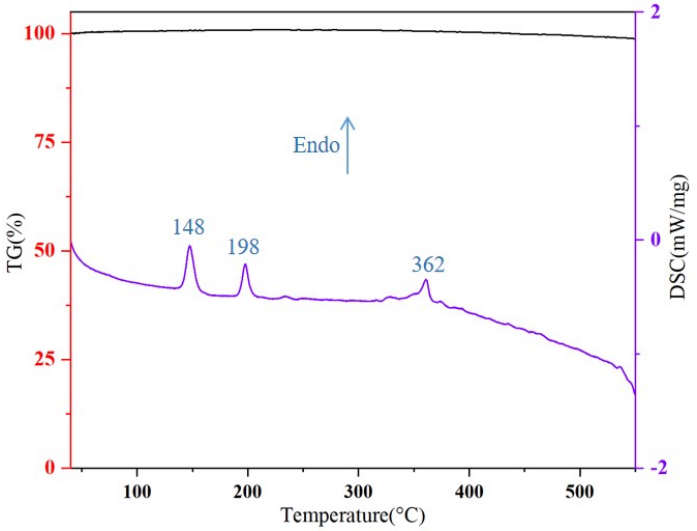

Figure S4. TG-DSC curves of $KRb_2(NO_3)_2Cl$.

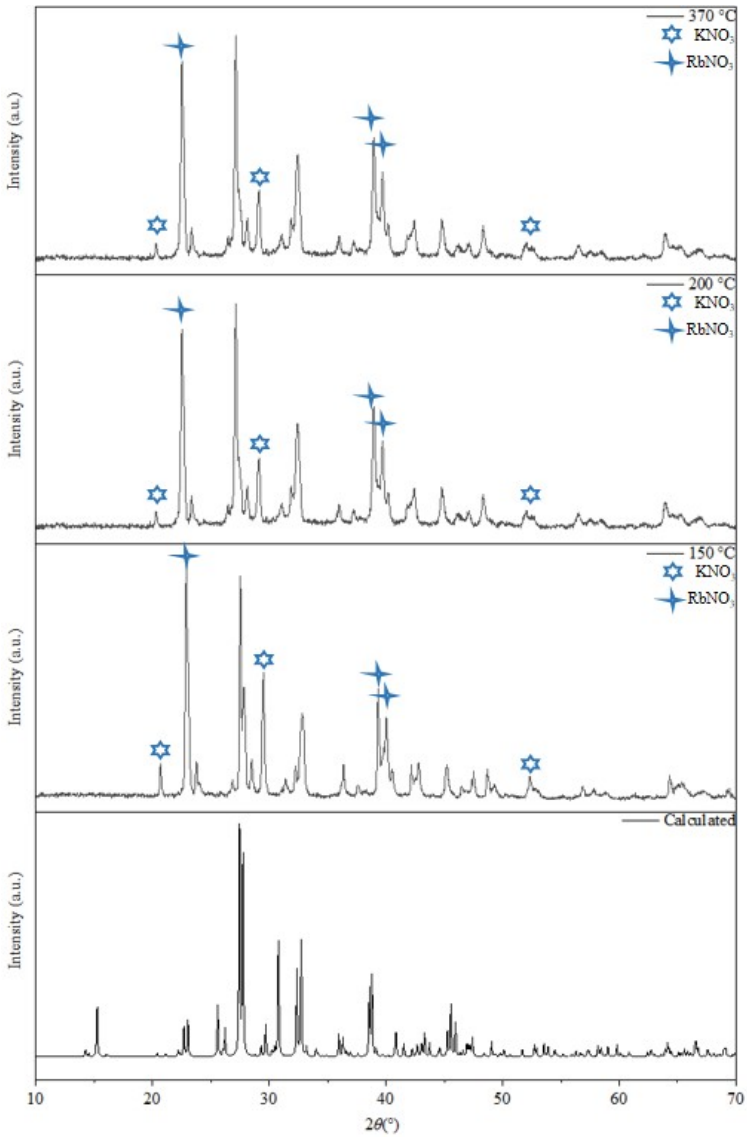

Figure S5. Experimental and calculated powder XRD patterns, for $KRb_2(NO_3)_2Cl$.

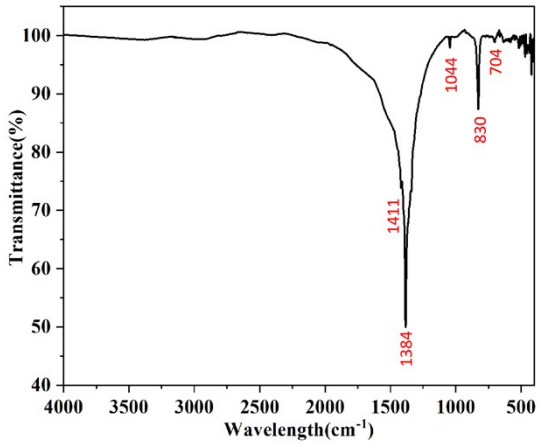

Figure S6. The IR spectrum for $KRb_2(NO_3)_2Cl$.

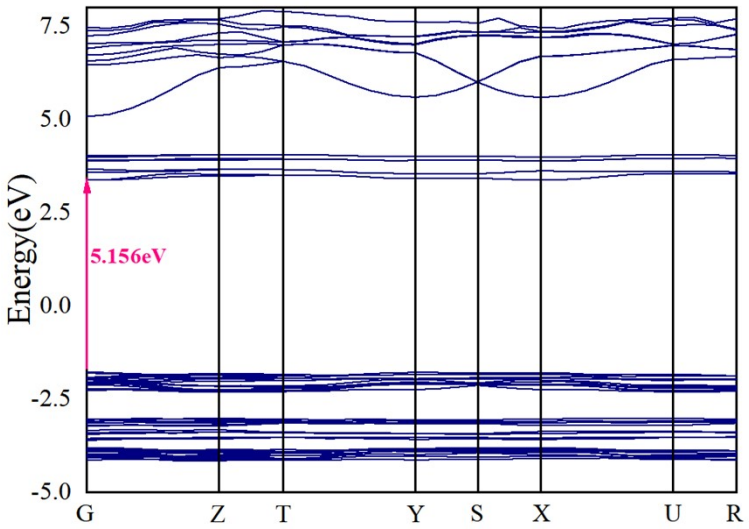

Figure S7. The HSE06 band structures for $KRb_2(NO_3)_2Cl$.

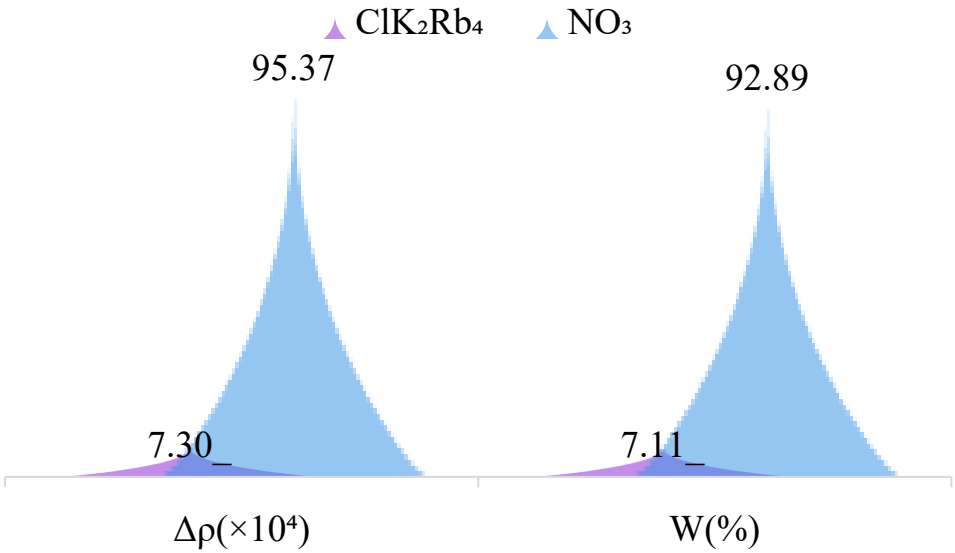

Figure S8. Bonding electron density difference ($\Delta\rho$) and contribution percent *w* (%) of different units in $KRb_2(NO_3)_2Cl$ calculated by the REDA method.