Table S1. Crystal data and structure refinement for $K_2NbO_2F_3$

Formula	$K_2NbO_2F_3$
Formula weight	260.11
Crystal system	orthorhombic
Space group, Z	$Pna2_1$, 4
a, Å	7.6269(2)
b, Å,	11.8526(4)
c, Å	5.70105(16)
V, Å^3	515.37(3)
D_x, g/см^3	3.352
Wavelength, Å	Mo-K_α; 0.71073
μ, мм$^{-1}$	3.919
θ_{max}, range/degree	3.18-30.67
Refl. collected/unique/R_{int}	7876 / 1508 / 1366 / 4.66
Completeness to Θ, %	0.974
Parameters	73
GOF (S)	1.110
R_{all}, R_{gt}, R_{wgt} [1]	0.0592, 0.0545, 0.1308
$\Delta\rho_{min}/\Delta\rho_{max}$, э/ Å^3	-4.756 / 0.879

[1] $R_{gt} = \Sigma. \, ||F_o| - |F_c|| = \Sigma \, |F_o|$ and $R_{wgt} = [\Sigma \, w \, (F_o^2 - F_c^2)^2 / \Sigma \, w \, (F_o^2)^2]^{1/2}$ *for* $F_o^2 > 2\sigma(F_o^2)$.

Table S2. Atomic coordinates and equivalent displacement parameters for. $K_2NbO_2F_3$

Atom	***x/a***	***y/b***	***z/c***	U_{equ}, Å^2
Nb	0.13928(5)	0.06229(3)	0.4861(7)	0.0098(2)
K1	-0.0124(2)	0.2401(1)	0.985(1)	0.0192(3)
K2	0.1434(1)	0.4175(1)	0.486(2)	0.0220(3)
O1	-0.001(3)	-0.005(2)	0.736(3)	0.0199(10)
O2	0.0432(6)	0.1991(3)	0.494(3)	0.0260(11)
F1	0.2809(4)	-0.0921(3)	0.491(3)	0.0240(8)
F2	0.3250(15)	0.1038(10)	0.7209(9)	0.021(2)
F3	0.3211(16)	0.1060(12)	0.2495(9)	0.029(3)

Table S3. Interatomic distances for $K_2NbO_2F_3$.

Bond	**Distance, Å**	**Bond**	**Distance, Å**
Nb – O2	1.780(4)	Nb- F2	2.010(8)
Nb – O1	1.900(17)	Nb- F1	2.125(3)
Nb– O1`	1.951(17)	**av.Nb-F**	2.045
Nb– F3	2.003(9)	**av. Nb – O**	1.879
K1 – F1	2.660(3)	**K2** – F2	2.686(11)
K1– F3	2.686(10)	K2– O2	2.700(5)

K1 – F2	2.688(10)	K2 – F3	2.706(14)
K1 – F1`	2.697(4)	K2 – F2`	2.785(13)
K1- O2	2.87(2)	K2- F3`	2.817(14)
K1-O2`	2.98(2)	K2-F1	2.881(17)
K1- O1	3.14(2)	K2- F1`	2.940(17)
K1-O1`	3.23(2)	K2-O1	3.21(2)
av. K1 – O	3.054	K2-O1`	3.24(2)
av. K1- F	2.683	**Av. K2 – O**	3.048
		Av.. K2- F	2.803