Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

$NaVSeO_5$: Synergistic Combinations to Excellent Birefringent Materials

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Content

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for nNaVSeO$_5$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	x/a	y/b	z/c	U(eq)	BVS
Na(1)	7368(2)	857(7)	1272(2)	23(1)	1.023
V(1)	9091(1)	5725(2)	1349(1)	9(1)	5.035
Se(1)	9223(1)	2085(1)	3896(1)	9(1)	3.955
O(1)	9242(2)	-46(10)	1388(3)	13(1)	1.852
O(2)	9501(2)	4997(9)	3036(3)	11(1)	2.042
O(3)	8139(2)	5350(10)	981(3)	16(1)	2.011
O(4)	9138(2)	5246(10)	4850(3)	13(1)	2.018
O(5)	8278(2)	1307(10)	3147(3)	14(1)	2.090

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

[b] Bond valence sums (BVS) are calculated by using the bond-valence model (S_i = exp [(R_o−R_i / B], where R_o is an empirical constant, R_i is the length of bond *i* (in angstroms), and B = 0.37 Å)

Table S2. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $NaVSeO_5$. The anisotropic displacement factor exponent takes the form: $2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Na(1)	22(1)	27(1)	17(1)	3(1)	4(1)	-8(1)
V(1)	14(1)	7(1)	8(1)	0(1)	6(1)	0(1)
Se(1)	13(1)	7(1)	9(1)	0(1)	5(1)	0(1)
O(1)	18(2)	11(2)	9(2)	0(1)	3(2)	1(2)
O(2)	17(2)	9(2)	7(2)	0(1)	6(2)	-1(2)
O(3)	16(2)	17(2)	16(2)	3(2)	7(2)	0(2)
O(4)	16(2)	12(2)	12(2)	-1(2)	7(2)	-1(2)
O(5)	14(2)	15(2)	13(2)	-1(2)	4(2)	-2(2)

Table S3. Selected bond lengths (Å) and angles (°) for $NaVSeO_5$.

Na(1)-O(3)	2.339(4)	V(1)-O(1)	2.230(4)
Na(1)-O(3)#1	2.631(5)	V(1)-O(2)#6	2.398(4)
Na(1)-O(3)#4	2.639(5)	V(1)-O(2)	1.956(4)
Na(1)-O(4)#2	2.572(5)	V(1)-O(3)	1.625(4)
Na(1)-O(5)#2	2.367(4)	V(1)-O(4)#7	1.932(4)
Na(1)-O(5)#3	2.632(5)	Se(1)-O(2)	1.750(3)
Na(1)-O(5)	2.293(5)	Se(1)-O(4)	1.743(4)
V(1)-O(1)#5	1.644(4)	Se(1)-O(5)	1.644(4)
O(3)-Na(1)-O(3)#1	87.32(15)	O(5)#2-Na(1)-O(5)#3	100.17(15)
O(3)#1-Na(1)-O(3)#4	72.69(15)	O(1)#5-V(1)-O(1)	164.2(2)
O(3)-Na(1)-O(3)#4	100.74(16)	O(1)#5-V(1)-O(2)#6	87.64(16)
O(3)-Na(1)-O(4)#2	124.34(16)	O(1)-V(1)-O(2)#6	76.65(13)
O(3)-Na(1)-O(5)#3	79.30(15)	O(1)#5-V(1)-O(2)	96.81(17)
O(3)-Na(1)-O(5)#2	171.59(18)	O(1)#5-V(1)-O(4)#7	98.63(17)
O(3)#1-Na(1)-O(5)#3	114.78(15)	O(2)-V(1)-O(1)	80.88(14)
O(4)#2-Na(1)-O(3)#4	111.55(15)	O(2)-V(1)-O(2)#6	73.55(15)
O(4)#2-Na(1)-O(3)#1	62.55(12)	O(3)-V(1)-O(1)#5	104.2(2)
O(4)#2-Na(1)-O(5)#3	74.00(14)	O(3)-V(1)-O(1)	91.60(17)
O(5)-Na(1)-O(3)#1	156.54(17)	O(3)-V(1)-O(2)#6	168.03(17)
O(5)-Na(1)-O(3)#4	88.98(15)	O(3)-V(1)-O(2)	102.69(17)
O(5)#2-Na(1)-O(3)#4	78.67(14)	O(3)-V(1)-O(4)#7	98.45(18)

O(5)#2-Na(1)-O(3)#1	100.41(15)	O(4)#7-V(1)-O(1)	77.20(14)
O(5)-Na(1)-O(3)	81.74(16)	O(4)#7-V(1)-O(2)	149.81(16)
O(5)#3-Na(1)-O(3)#4	172.47(16)	O(4)#7-V(1)-O(2)#6	81.33(14)
O(5)#2-Na(1)-O(4)#2	62.99(14)	O(4)-Se(1)-O(2)	95.27(17)
O(5)-Na(1)-O(4)#2	140.04(16)	O(5)-Se(1)-O(2)	104.83(18)
O(5)-Na(1)-O(5)#2	89.86(15)	O(5)-Se(1)-O(4)	99.50(18)
O(5)-Na(1)-O(5)#3	83.57(15)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,-y+1/2,-z	#2 -x+3/2,y-1/2,-z+1/2	#3 -x+3/2,y+1/2,-z+1/2
#4 x,y-1,z	#5 x,y+1,z	#6 -x+2,y,-z+1/2
#7 x,-y+1,z-1/2	#8 x,-y+1,z+1/2	

Table S4. Previously reported partial bond lengths (Å) and angles (°) for vanadium selenates.

		KV_2SeO_7	
V(1)-O(2)×2	1.640(9)	V(2)-O(2)×2	1.952(8)
V(1)-O(3)	1.802(9)	V(2)-O(1)	2.192(9)
V(2)-O(5)	1.603(9)	Se(1)-O(3)	1.732(10)
V(1)-O(1)	1.643(9)	Se(l)-O(4)×2	1.669(6)
V(2)-O(4)×2	2.012(8)	O(2)-V(l)-O(l)	111.4(3)
O(2)-V(1)-O(2)	108.6(8)	O(1)-V(1)-O(3)	107.9(5)
O(2)-V(1)-O(3)	108.8(4)	O(2)-V(2)-O(2)	87.3(7)
O(5)-V(2)-O(2)	99.7(4)	O(2)-V(2)-O(4)	90.5(4)
O(5)-V(2)-O(4)	94.9(3)	O(5)-V(2)-O(1)	175.2(5)
O(4)-V(2)-O(4)	87.9(4)	O(4)-V(2)-O(1)	81.6(3)
O(2)-V(2)-O(1)	83.8(3)	O(4)-Se-O(3)	95.7(3)
V(1)-O(2)-V(2)	166.1(6)	O(4)-Se-O(4)	100.5(5)
		$Sr(VO_2F)(SeO_3)$	
V(1)-O(5)	1.618(3)	V(1)-O(4)#4	2.304(3)
V(1)-O(4)	1.667(3)	Se(1)-O(1)	1.651(3)
V(1)-O(2)#3)	1.968(3)	Se(1)-O(3)	1.736(3)
V(1)-O(3)#7	1.969(3)	Se(1)-O(2)	1.747(3)
O(1)-Se(1)-O(3)	103.24(13)	O(5)-V(1)-O(4)	105.73(13)
O(1)-Se(1)-O(2)	100.75(13)	O(5)-V(1)-O(2)#1	99.61(14)
O(3)-Se(1)-O(2)	102.69(13)	O(4)-V(1)-O(2)#1	96.28(13)

O(5)-V(1)-O(3)#3	100.56(13)	O(2)#1-V(1)-O(3)#3	154.43(11)
O(4)-V(1)-O(3)#3	93.21(12)	O(5)-V(1)-O(4)#2	171.46(12)
O(4)-V(1)-O(4)#2	82.76(11)	O(2)#1-V(1)-O(4)#2	79.98(11)
O(3)#3-V(1)-O(4)#2	77.74(11)		

$Ba(VO_2F)(SeO_3)$

V(1)-O(4)	1.623(3)	V(1)-O(2)#5	2.304(3)
V(1)-O(2)	1.664(3)	Se(1)-O(1)	1.648(3)
V(1)-O(3)	1.976(3)	Se(1)-O(5)	1.734(3)
V(1)-O(5)#5	1.972(3)	Se(1)-O(3)	1.740(3)
O(1)-Se(1)-O(5)	103.05(15)	O(1)-Se(1)-O(3)	101.04(14)
O(5)-Se(1)-O(3)	102.90(14)	O(4)-V(1)-O(2)	104.86(15)
O(4)-V(1)-O(3)	98.27(14)	O(2)-V(1)-O(3)	95.99(13)
O(4)-V(1)-O(5)#1	102.98(13)	O(2)-V(1)-O(5)#1	93.96(13)
O(3)-V(1)-O(5)#1	153.34(12)	O(4)-V(1)-O(2)#1	172.25(14)
O(2)-V(1)-O(2)#1	82.59(12)	O(3)-V(1)-O(2)#1	78.52(11)
O(5)#1-V(1)-O(2)#1	78.33(10)		

Table S5. Comparison of birefringence in some crystals

No	Compounds	Space group	Cutoff edge	Δn
1	YVO_4	$I4_1/amd$	400 nm	0.208 @1064 nm
2	$LiNbO_3$	$R3c$	420 nm	0.074@546 nm
3	TiO_2	$P42/mnm$	400 nm	0.256@1530 nm
4	Li_3VO_4	$Pmn2_1$	290 nm	Cal 0.01@500-1100 nm
5	β-Tl_3VO_4	$Imm2$	401 nm	Cal 0.057 @1064 nm
6	$LiNaV_2O_6$	$C2/c$	385 nm	Cal 0.137 @546 nm
7	$Ca_3V_2O_8$	$R3c$	349 nm	0.023 @546 nm
8	$NaCa_4V_5O_{17}$	$P\bar{1}$	345 nm	Cal 0.1 @1064 nm
9	$Cs_2Zn_4V_4O_{15}$	$C2/c$	372 nm	Cal 0.014@1064 nm
10	$NaVSeO_5$	$C2/c$	336nm	0.180@546 nm

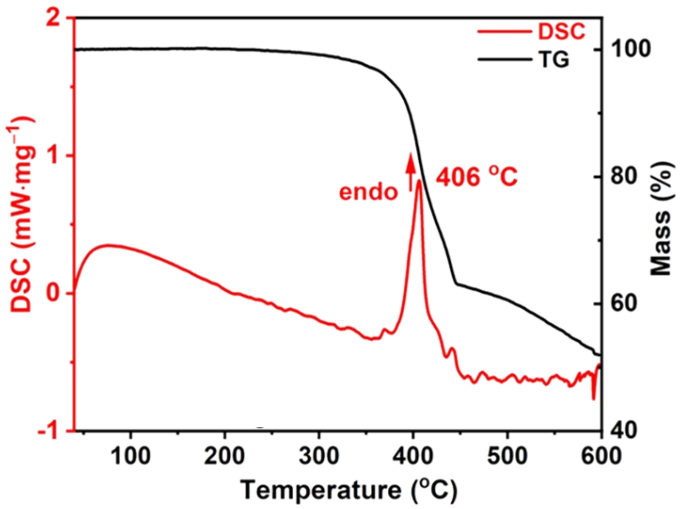

Figure S1. Thermal properties of TG-DSC curves of $NaVSeO_5$

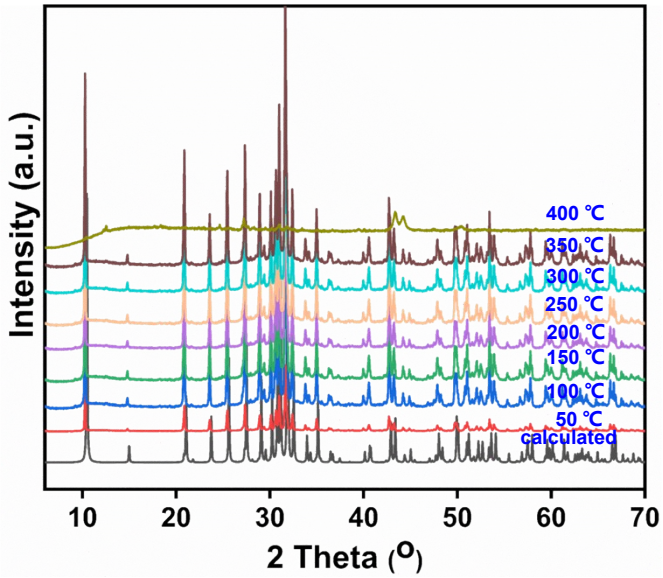

Figure S2. Powder X-ray diffraction patterns of annealing experiments on $NaVSeO_5$.

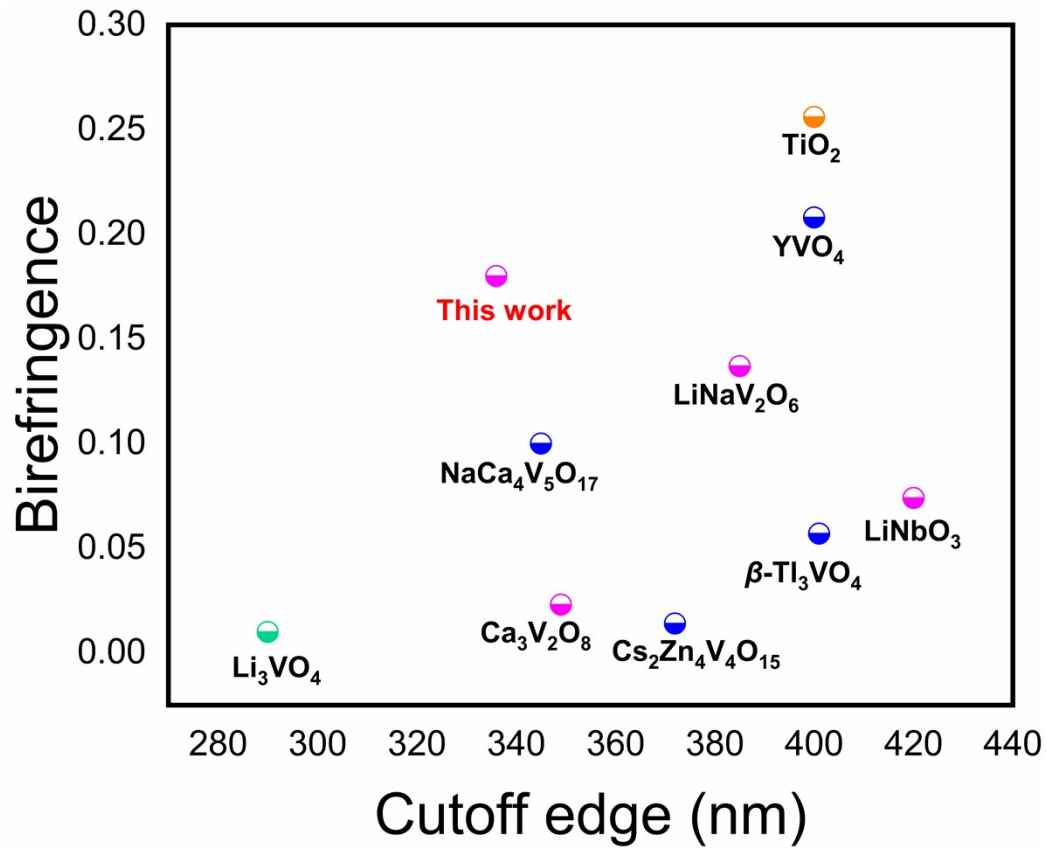

Figure S3. Comparison of birefringence in some crystals