Supporting Information

A new noncentrosymmetric vanadoborate: synthesis, crystal structure and characterization of $K_2SrVB_5O_{12}$

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Figure S1. The coordination of K atoms. The green ones are K(1) atoms, and the blue ones are K(2) atoms.

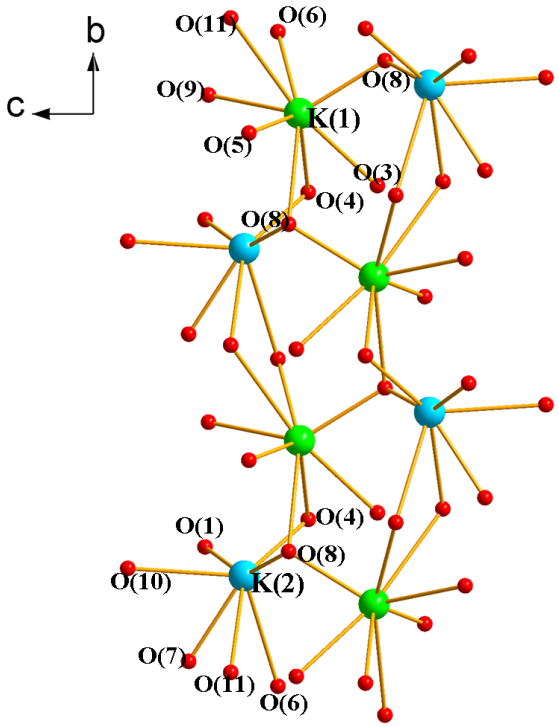

Figure S2. The coordination of Sr atoms.

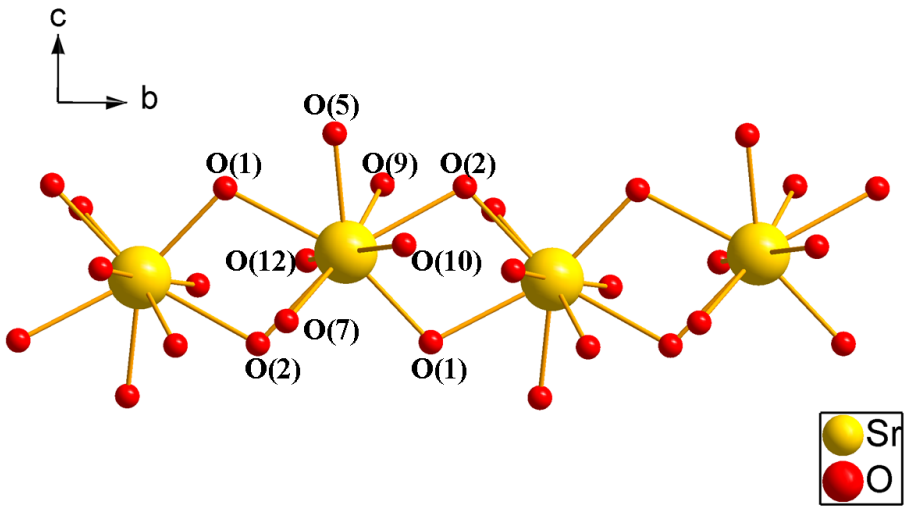

Figure S3. UV-Vis-NIR Diffuse-reflectance Spectrum of $K_2SrVB_5O_{12}$.

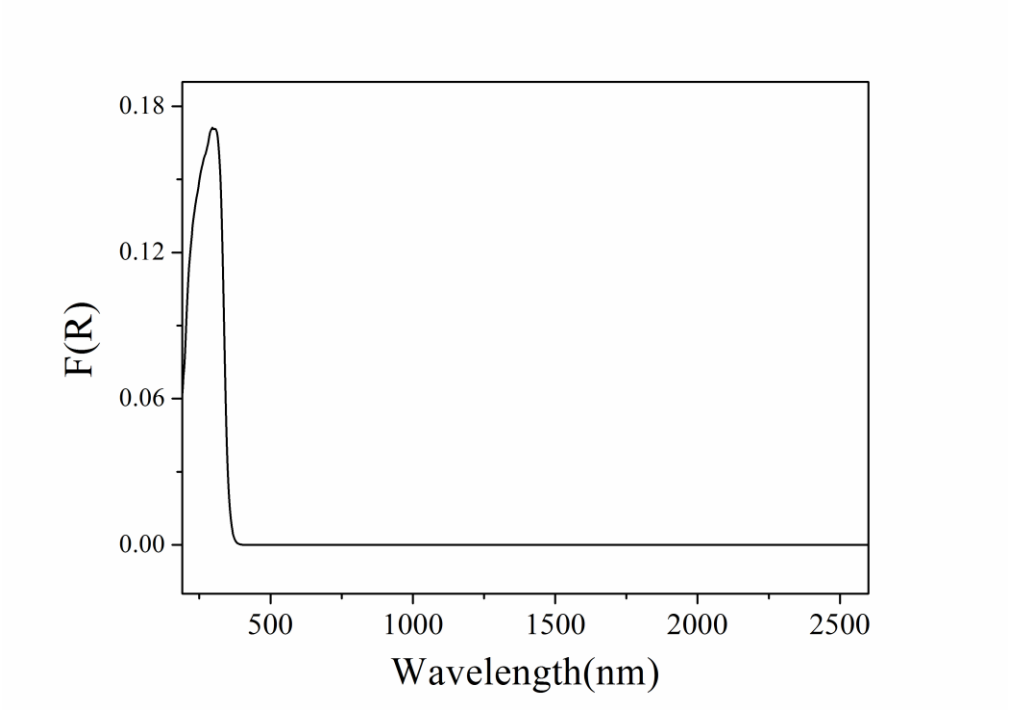

Figure S4. XRD patterns of $K_2SrVB_5O_{12}$.

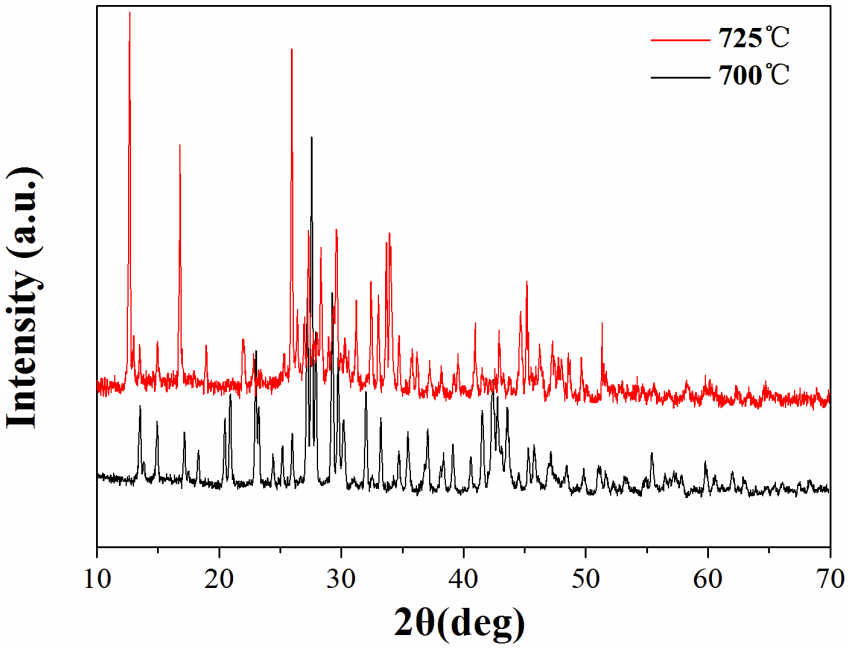

Figure S5. Absorption spectrum of $K_2SrVB_5O_{12}$.

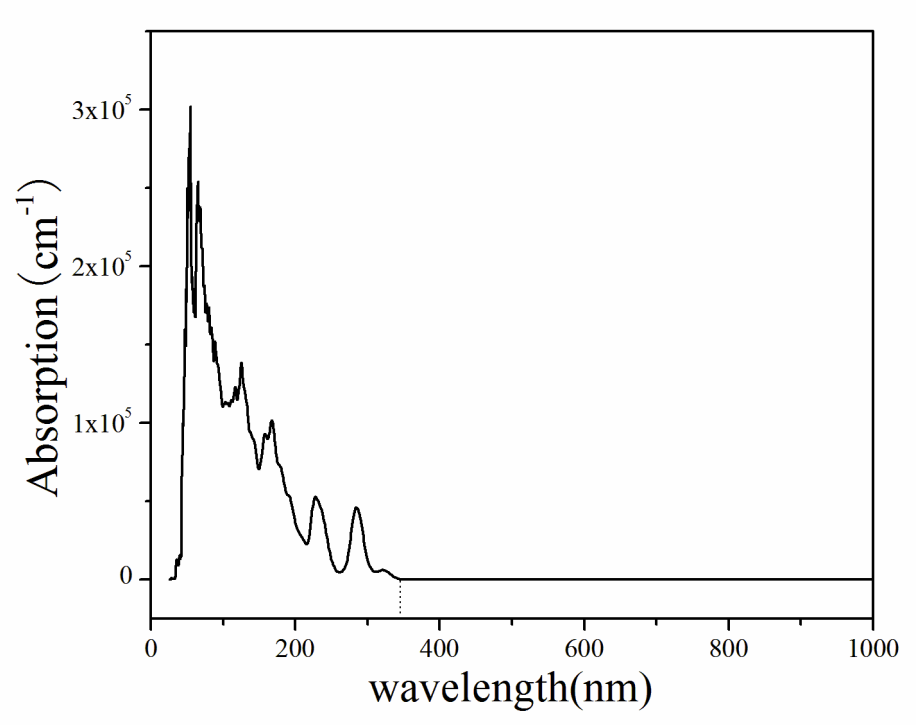

Table S1. Selected bond distances (Å) and angles (deg) for $K_2SrVB_5O_{12}$.

Sr(1)-O(5)	2.499(6)	K(2)-O(4)#9	2.785(7)
Sr(1)-O(1)#1	2.556(7)	K(2)-O(1)#9	2.955(7)
Sr(1)-O(7)	2.571(6)	K(2)-O(10)	2.986(7)
Sr(1)-O(9)#1	2.607(6)	K(2)-O(11)	2.993(7)
Sr(1)-O(2)	2.623(7)	K(2)-O(6)#5	3.134(7)
Sr(1)-O(10)#2	2.773(6)	B(1)-O(7)	1.459(11)
Sr(1)-O(2)#1	2.782(7)	B(1)-O(9)	1.466(12)
Sr(1)-O(1)	2.799(7)	B(1)-O(6)#10	1.469(11)
Sr(1)-O(12)#1	2.902(6)	B(1)-O(2)	1.483(11)
V(1)-O(8)	1.629(7)	B(2)-O(12)	1.340(12)
V(1)-O(5)	1.661(8)	B(2)-O(10)	1.356(11)
V(1)-O(1)	1.692(7)	B(2)-O(9)	1.401(11)
V(1)-O(4)	1.861(6)	B(3)-O(11)#2	1.452(12)
K(1)-O(8)	2.569(8)	B(3)-O(12)#2	1.453(12)
K(1)-O(5)#5	2.629(6)	B(3)-O(7)	1.456(11)
K(1)-O(6)	2.772(6)	B(3)-O(10)	1.519(11)
K(1)-O(3)	2.862(6)	B(4)-O(11)	1.338(12)
K(1)-O(9)#6	2.888(7)	B(4)-O(2)#11	1.369(11)
K(1)-O(4)#7	3.151(7)	B(4)-O(3)	1.396(12)
K(1)-O(11)#4	3.163(7)	B(5)-O(6)	1.334(11)
K(1)-O(8)#5	3.224(8)	B(5)-O(3)#12	1.366(11)
K(2)-O(8)	2.541(8)	B(5)-O(4)	1.367(11)
K(2)-O(7)#8	2.639(6)	O(11)#2-B(3)-O(7)	108.3(7)
O(7)-B(1)-O(9)	108.5(7)	O(12)#2-B(3)-O(7)	112.6(8)
O(7)-B(1)-O(6)#10	113.3(7)	O(11)#2-B(3)-O(10)	109.8(8)
O(9)-B(1)-O(6)#10	109.8(7)	O(12)#2-B(3)-O(10)	104.2(7)
O(7)-B(1)-O(2)	107.0(7)	O(7)-B(3)-O(10)	110.2(7)
O(9)-B(1)-O(2)	107.6(7)	O(11)-B(4)-O(2)#11	124.1(9)

O(6)#10-B(1)-O(2)	110.4(7)	O(11)-B(4)-O(3)	116.7(8)
O(12)-B(2)-O(10)	125.7(9)	O(2)#11-B(4)-O(3)	119.2(9)
O(12)-B(2)-O(9)	112.7(8)	O(6)-B(5)-O(3)#12	121.2(9)
O(10)-B(2)-O(9)	121.6(9)	O(6)-B(5)-O(4)	122.7(8)
O(11)#2-B(3)-O(12)#2	111.7(8)	O(3)#12-B(5)-O(4)	116.1(7)

Symmetry transformations used to generate equivalent atoms:

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

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

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

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

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