Supporting Information

Synthesis and Characterization of $Cs_2Zn_4V_4O_{15}$ - a New Vanadate in the Cs-Zn-V-O Quaternary System

Qiuyuan Feng, Jianyi Zuo, and Hong Du *

College of Chemistry and Chemical Engineering, Xinjiang Normal University, Urumqi, Xinjiang 830054, P. R. China.

*E-mails: 175790509@qq.com (Hong Du);

Content

CCDC number: 2236458

Table S1. Atomic coordinates and equivalent isotropic displacement parameters and bond valence sum (BVS)* calculations for $Cs_2Zn_4V_4O_{15}$. *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atoms	x/a	y/b	z/c	U(eq)	BVS
Cs(1)	3759(1)	2560(1)	3234(1)	32(1)	0.925
Zn(1)	3386(1)	-2205(1)	6080(1)	15(1)	2.091
Zn(2)	4188(1)	2897(1)	5429(1)	16(1)	2.077
V(1)	5962(1)	7305(1)	3065(1)	16(1)	4.884
V(2)	3701(1)	-2350(1)	4556(1)	14(1)	4.849
O(1)	3611(2)	-3840(5)	5295(1)	19(1)	2.020
O(2)	6087(2)	8890(5)	3815(1)	20(1)	2.054
O(3)	3816(2)	758(5)	4685(2)	27(1)	1.973
O(4)	4574(2)	-3545(6)	4314(2)	24(1)	1.958
O(5)	6771(2)	7959(7)	2734(2)	37(1)	1.913
O(6)	5930(2)	4200(5)	3207(2)	26(1)	1.921
O(7)	2834(2)	-2941(6)	3939(2)	24(1)	1.958
O(8)	5000	8297(9)	2500	41(1)	2.059

(BVS)*：The bond valence sums were calculated using the formula $V_i=\sum S_{ij}=\sum\exp[(r_0-r_{ij})/B]$, where S_{ij} is the bond valence associated with bond length r_{ij}, and r_0 and B (usually 0.37) are empirically determined parameters.[1]

Table S2. Optimized atomic coordinates and equivalent isotropic displacement parameters and bond valence sum (BVS)* calculations for $Cs_2Zn_4V_4O_{15}$. *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atoms	x/a	y/b	z/c	U(eq)	BVS
Cs(1)	3706	2462.6	3149	32.13	1.173
Zn(1)	3391	-2277.5	6081	15.23	1.681
Zn(2)	4208.5	2922.3	5348.2	16.47	1.653
V(1)	5921.5	7275.3	3076.8	16.19	4.401
V(2)	3671.4	-2490.3	4476.1	13.49	4.405
O(1)	3452.2	-3878.7	5202.5	18.79	1.736
O(2)	6074.6	8821.6	3848.8	20.43	1.799
O(3)	3872	672.1	4574.9	27.43	1.773
O(4)	4558.2	-4035	4294.5	24.34	1.726
O(5)	6789.9	7712.9	2750.1	37.03	1.789
O(6)	5772.6	4126.7	3194.9	26.35	1.758
O(7)	2831.1	-2935.8	3799.6	24.4	1.745
O(8)	5000	8583.6	2500	40.91	1.973

(BVS)*：The bond valence sums were calculated using the formula $V_i=\sum S_{ij}=\sum \exp[(r_0-r_{ij})/B]$, where S_{ij} is the bond valence associated with bond length r_{ij}, and r_0 and B (usually 0.37) are empirically determined parameters.[1]

Table S3. The selected bond lengths and angles of $Cs_2Zn_4V_4O_{15}$.

Cs(1)-O(3)	3.168(3)	Zn(1)-O(7)#8	1.912(3)
Cs(1)-O(4)#2	3.137(3)	Zn(2)-O(1)#2	1.961(3)
Cs(1)-O(5)#3	3.081(4)	Zn(2)-O(2)#6	1.976(3)
Cs(1)-O(5)#4	3.183(4)	Zn(2)-O(3)	1.917(3)
Cs(1)-O(5)#1	3.525(4)	Zn(2)-O(4)#7	1.935(3)
Cs(1)-O(6)	3.537(3)	V(1)-O(2)	1.758(3)
Cs(1)-O(6)#1	3.278(3)	V(1)-O(5)	1.613(4)
Cs(1)-O(7)	3.728(3)	V(1)-O(6)	1.692(3)
Cs(1)-O(7)#2	3.320(3)	V(1)-O(8)	1.7855(16)
Cs(1)-O(8)#5	3.561(3)	V(2)-O(1)	1.773(3)
Zn(1)-O(1)	1.959(3)	V(2)-O(3)	1.689(3)
Zn(1)-O(2)#6	1.951(3)	V(2)-O(4)	1.689(3)
Zn(1)-O(6)#7	1.956(3)	V(2)-O(7)	1.691(3)
O(3)-Cs(1)-O(5)#4	108.84(9)	O(6)-Cs(1)-O(7)	131.57(7)
O(3)-Cs(1)-O(5)#1	138.98(8)	O(6)#1-Cs(1)-O(7)	136.44(7)
O(3)-Cs(1)-O(6)#1	169.85(8)	O(6)#1-Cs(1)-O(7)#2	112.42(8)
O(3)-Cs(1)-O(6)	105.38(8)	O(6)-Cs(1)-O(8)#5	62.03(7)
O(3)-Cs(1)-O(7)#2	73.70(8)	O(6)#1-Cs(1)-O(8)#5	64.50(7)
O(3)-Cs(1)-O(7)	46.57(7)	O(7)#2-Cs(1)-O(5)#1	65.69(8)
O(3)-Cs(1)-O(8)#5	108.32(7)	O(7)#2-Cs(1)-O(6)	110.15(7)
O(4)#2-Cs(1)-O(3)	65.81(8)	O(7)#2-Cs(1)-O(7)	98.72(8)
O(4)#2-Cs(1)-O(5)#4	169.26(9)	O(7)#2-Cs(1)-O(8)#5	172.14(7)
O(4)#2-Cs(1)-O(5)#1	82.94(9)	O(8)#5-Cs(1)-O(7)	87.80(7)
O(4)#2-Cs(1)-O(6)#1	111.42(8)	O(2)#6-Zn(1)-O(1)	110.55(12)
O(4)#2-Cs(1)-O(6)	66.57(7)	O(2)#6-Zn(1)-O(6)#7	105.15(12)
O(4)#2-Cs(1)-O(7)	111.96(8)	O(6)#7-Zn(1)-O(1)	103.03(12)
O(4)#2-Cs(1)-O(7)#2	49.25(7)	O(7)#8-Zn(1)-O(1)	111.38(13)
O(4)#2-Cs(1)-O(8)#5	124.12(6)	O(7)#8-Zn(1)-O(2)#6	111.39(13)
O(5)#3-Cs(1)-O(3)	99.29(9)	O(7)#8-Zn(1)-O(6)#7	114.89(14)
O(5)#3-Cs(1)-O(4)#2	115.07(9)	O(1)#2-Zn(2)-O(2)#6	111.72(12)
O(5)#4-Cs(1)-O(5)#1	105.82(11)	O(3)-Zn(2)-O(1)#2	111.54(13)
O(5)#3-Cs(1)-O(5)#4	74.43(8)	O(3)-Zn(2)-O(2)#6	106.18(13)
O(5)#3-Cs(1)-O(5)#1	69.65(8)	O(3)-Zn(2)-O(4)#7	116.31(14)
O(5)#3-Cs(1)-O(6)#1	90.72(9)	O(4)#7-Zn(2)-O(1)#2	106.64(13)
O(5)#4-Cs(1)-O(6)	107.57(8)	O(4)#7-Zn(2)-O(2)#6	104.30(13)
O(5)#1-Cs(1)-O(6)	83.99(8)	O(2)-V(1)-O(8)	111.19(14)
O(5)#4-Cs(1)-O(6)#1	72.11(8)	O(5)-V(1)-O(2)	109.42(17)
O(5)#3-Cs(1)-O(6)	152.73(8)	O(5)-V(1)-O(6)	110.21(18)
O(5)#4-Cs(1)-O(7)#2	139.88(8)	O(5)-V(1)-O(8)	106.58(15)
O(5)#1-Cs(1)-O(7)	144.25(8)	O(6)-V(1)-O(2)	108.62(15)
O(5)#3-Cs(1)-O(7)	74.62(8)	O(6)-V(1)-O(8)	110.80(18)
O(5)#4-Cs(1)-O(7)	64.50(8)	O(3)-V(2)-O(1)	109.28(15)
O(5)#3-Cs(1)-O(7)#2	65.82(9)	O(3)-V(2)-O(7)	110.30(15)

O(5)#4-Cs(1)-O(8)#5	47.28(7)	O(4)-V(2)-O(1)	108.39(14)
O(5)#1-Cs(1)-O(8)#5	111.17(8)	O(4)-V(2)-O(3)	110.79(16)
O(5)#3-Cs(1)-O(8)#5	120.57(7)	O(4)-V(2)-O(7)	105.81(15)
O(6)#1-Cs(1)-O(5)#1	46.80(8)	O(7)-V(2)-O(1)	112.22(15)
O(6)#1-Cs(1)-O(6)	65.21(9)		

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z-1	#2 -x,y-1/2,-z+2	#3 x+1,y,z+1
#4 -x+1,y+1/2,-z+2	#5 x,y,z+1	#6 -x+1,y-1/2,-z+2
#7 -x,y-1/2,-z+1	#8 -x,y+1/2,-z+2	#9 x-1,y,z
#10 x,y,z-1	#11 -x,y+1/2,-z+1	#12 x+1,y,z

Table S4 Vanadate containing Cs and Zn ions. Note the following compounds are all from ICSD and the anionic group is the $[VO_x]$ group, except for other disordered structures, fluorides, and structures containing crystalline water, all cesium vanadate and zinc vanadate are summarized.

No.	Compounds	Dimension	Basic Units	Space group	Ref
1	$Cs_3Mn_3V_4O_{16}$	0D	$[VO_4]$	$P\bar{1}$	2
2	Cs_2LiVO_4	0D	$[VO_4]$	$Cmc2_1$	3
3	Cs_2NaVO_4	0D	$[VO_4]$	$P2_1/m$	4
4	$Cs_2(UO_2)_2V_2O_8$	0D	$[VO_5]$	$P2_1/c$	5
5	$CsSbV_2O_8$	0D	$[VO_4]$	$P2_1/c$	6
6	$K_2CsLa(VO_4)_2$	0D	$[VO_4]$	$P2_1/m$	7
7	$CsVO_3$	0D	$[VO_4]$	$P6_3/m$	8
8	$Cs_2Sr(VO_3)_4$	0D	$[VO_4]$	$P4/mmm$	9
9	$CsNbV_2O_8$	0D	$[VO_4] + [V_2O_7]$	$P2_1/m$	10
10	$CsTaV_2O_8$	0D	$[VO_4] + [V_2O_7]$	$P2_1/m$	10
11	$Cs_2Sr(VO_3)_4$	0D	$[V_4O_{12}]$	$P4/nbm$	11
12	$Cs_{11}(Ge_9)_2VO_4$	0D	$[VO_4]$	$P2_1/c$	12
13	$Cs_2CaV_2O_7$	0D	$[V_2O_7]$	$P2_1/c$	13

14	$CsVO_3$	1D	$[VO_4]$	*Pbcm*	14
15	$Cs_2FeV_6O_{16}$	2D	$[VO_4]$	$P\bar{1}$	15
16	$Cs_2V_5O_{13}$	2D	$[VO_4] + [VO_5]$	*I*4*mm*	16
17	CsV_2O_5	2D	$[VO_4] + [VO_5]$	$P2_1/c$	17
18	CsV_3O_8	2D	$[VO_5] + [VO_6]$	$P2_1/m$	18
19	$Cs(UO_2)(VO_3)_3$	2D	$[VO_5]$	$P2_1/c$	19
20	$Cs_2V_3O_8$	2D	$[VO_4] + [VO_5]$	*P*4*bm*	20
21	$CsCrV_2O_7$	2D	$[VO_4]$	*P*2/*c*	21
22	$Cs_4V_8O_{22}$	2D	$[VO_4] + [VO_5]$	$Pca2_1$	22
23	$Cs_4Ba(VO_3)_6$	3D	$[VO_4]$	*R*3*c*	23
24	$Zn_2V_2O_7$	0D	$[V_2O_7]$	*C*2/*c*	24
25	$Zn_3(VO_4)_2$	0D	$[VO_4]$	*Cmca*	25
26	$SrZnV_2O_7$	0D	$[VO_4]$	$P2_1/c$	26
27	$CuZnV_2O_7$	0D	$[V_2O_7]$	*C*2/*c*	27
28	$Zn_4V_2O_9$	0D	$[V_2O_7]$	$P2_1$	28
29	$BaMgZn(VO_4)_2$	0D	$[VO_4]$	$I4_1/acd$	29

30	$Ca_5Mg_3Zn(VO_4)_6$	0D	$[VO_4]$	$I\bar{4}3d$	30
33	$Zn_2GaV_3O_{11}$	0D	$[VO_4] + [VO_5]$	$P\bar{1}$	31
32	$BaZnV_2O_7$	0D	$[V_2O_7]$	$P2_1/c$	32
33	$Ca_2NaZn_2(VO_4)_3$	0D	$[VO_4]$	$Ia\bar{3}d$	33
34	$Pb_2BaTeZn_3V_2O_{14}$	0D	$[VO_4]$	$P321$	34
35	$PbBa_2TeZn_3V_2O_{14}$	0D	$[VO_4]$	$P321$	34
36	$Na_2Zn_2Fe(VO_4)_3$	0D	$[VO_4]$	$C2/c$	35
37	$Na_2ZnV_2O_7$	0D	$[VO_4]$	$P\bar{4}21m$	36
38	$Ba_3Zn(V_2O_7)_2$	0D	$[V_2O_7]$	$P2_1/c$	37
39	$Pb_3Zn_3TeV_2O_{14}$	0D	$[VO_4]$	$P321$	38
40	$Ca_8BiZn(VO_4)_7$	0D	$[VO_4]$	$R3c$	39
41	$LiCa_3ZnV_3O_{12}$	0D	$[VO_4]$	$Ia\bar{3}d$	40
42	$Ag_2Zn_2Fe(VO_4)_3$	0D	$[VO_4]$	$C2/c$	41
43	$Ba_2ZnV_2O_8$	0D	$[VO_4]$	$P2_1/c$	42
44	$AgPb_2Zn_2(VO_4)_3$	0D	$[VO_4]$	$Ia\bar{3}d$	43
45	$Zn_3Fe_4(VO_4)_6$	0D	$[VO_4]$	$P\bar{1}$	26

46	$Ba_2Zn(VO_4)_2$	0D	$[VO_4]$	$P2_1/c$	44
47	$Ca_2AgZn_2V_3O_{12}$	0D	$[VO_4]$	$Ia\bar{3}d$	45
48	ZnV_3O_8	1D	$[VO_4]$	$P2_1/m$	46
49	$FeZn_2V_3O_{11}$	1D	$[VO_4]$	$P\bar{1}$	47
50	$MgZnV_2O_7$	1D	$[VO_4] + [VO_5]$	$C2/m$	48
51	$Ca_2Zn_2V_3O_{10}VO_4$	1D	$[VO_4] + [VO_5]$	$P2_1/c$	49
52	$PbZnV_2O_7$	1D	$[VO_4]$	$P2_1/c$	50
53	ZnV_2O_6	2D	$[VO_4]$	$C2$	51
54	$LiZnVO_4$	3D	$[VO_4]$	$R\bar{3}$	52
55	ZnV_3O_8	3D	$[VO_4] + [VO_5]$	$Iba2$	53

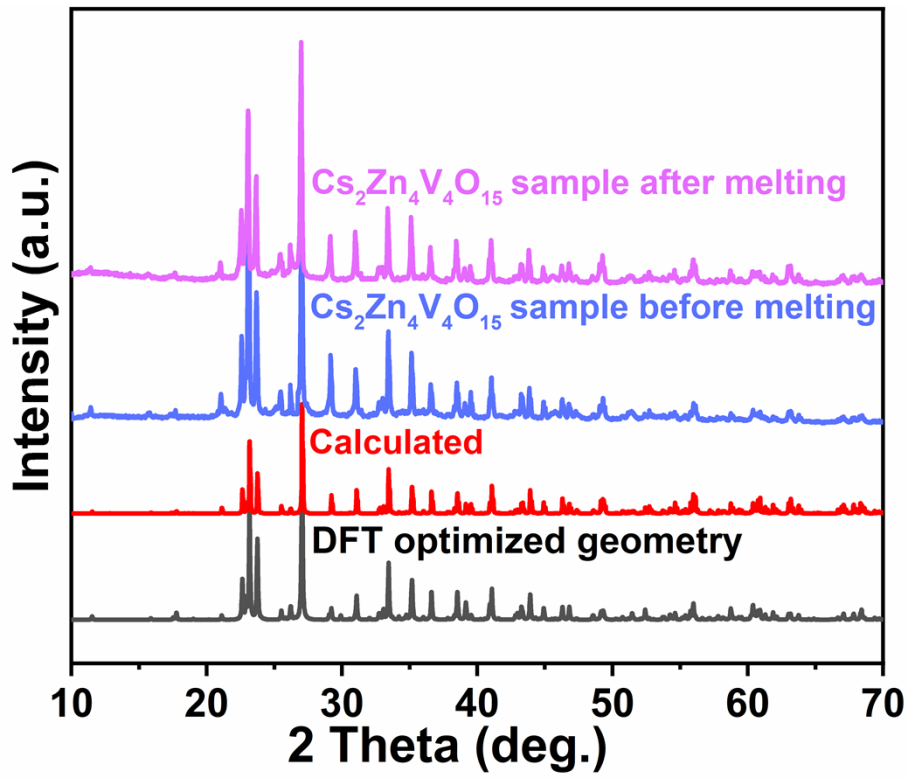

Figure S1. PXRD pattern calculated, before melting and after melting for $Cs_2Zn_4V_4O_{15}$

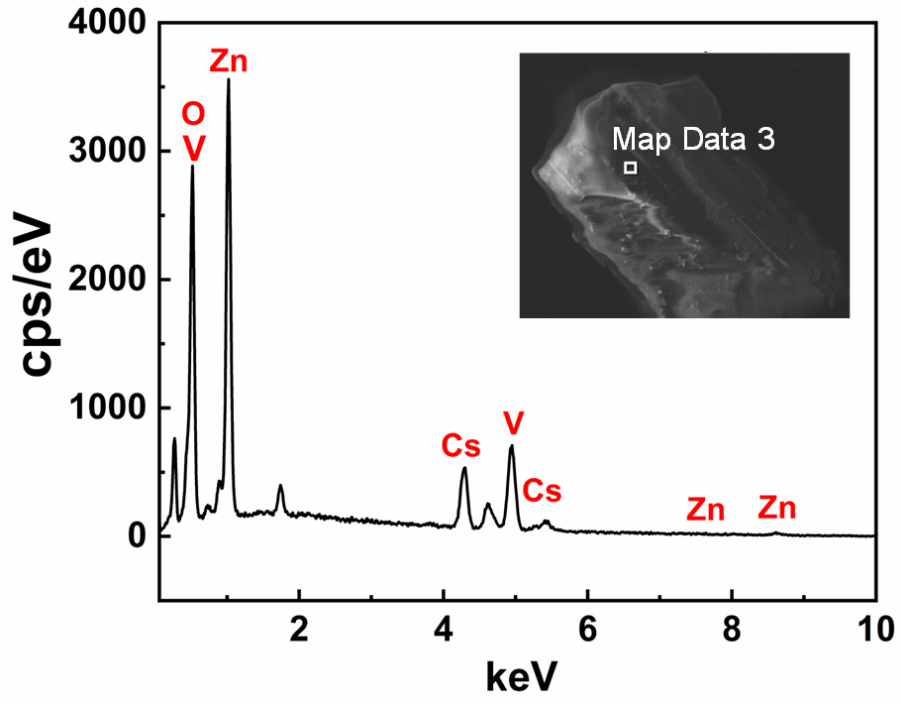

Figure S2. Energy dispersive X-ray spectroscope (EDS) analysis for $Cs_2Zn_4V_4O_{15}$.

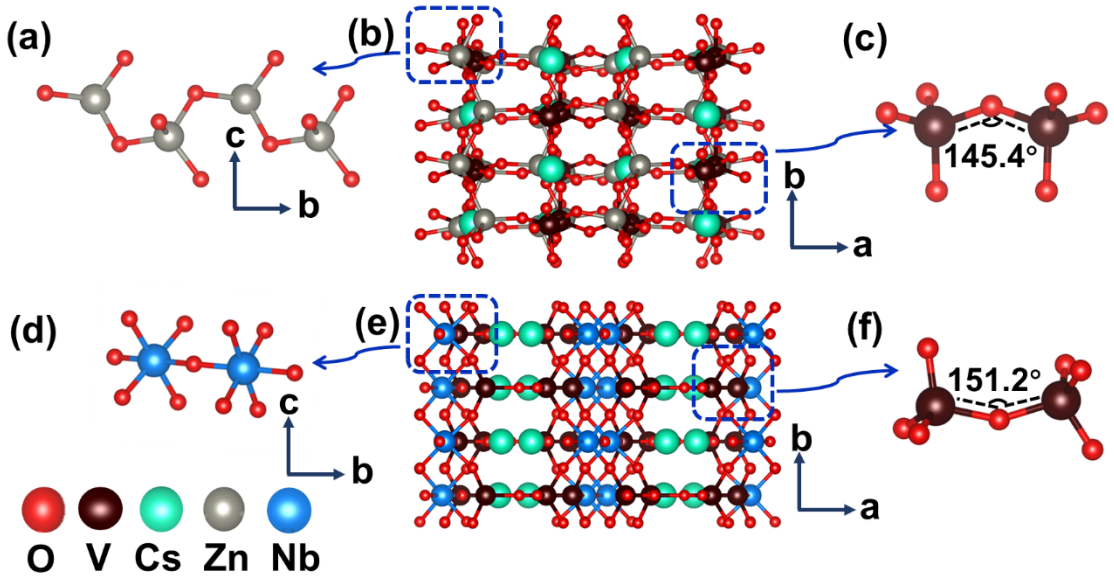

Figure S3 (a) $^{1}[ZnO_4]_{\infty}$ chain; (b) The crystal structure of $Cs_2Zn_4V_4O_{15;}$ (c) The V-O-V bond Angle is 145.4° in the $Cs_2Zn_4V_4O_{15}$ compound; (d) $[Nb_2O_{11}]$ dimer; (e) The crystal structure of $CsNbV_2O_{8;}$ (f) The V-O-V bond Angle is 151.2° in the $CsNbV_2O_{8;}$ compound; (O red; V brown; Cs:green; Zn gray; Nb:blue;)

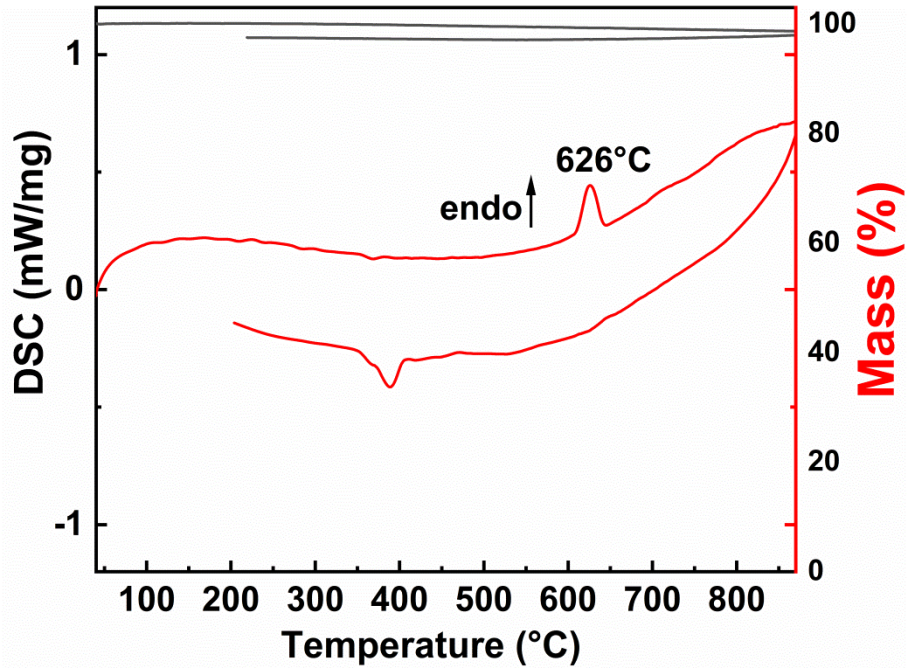

Figure S4. TG/DSC curves of $Cs_2Zn_4V_4O_{15}$.

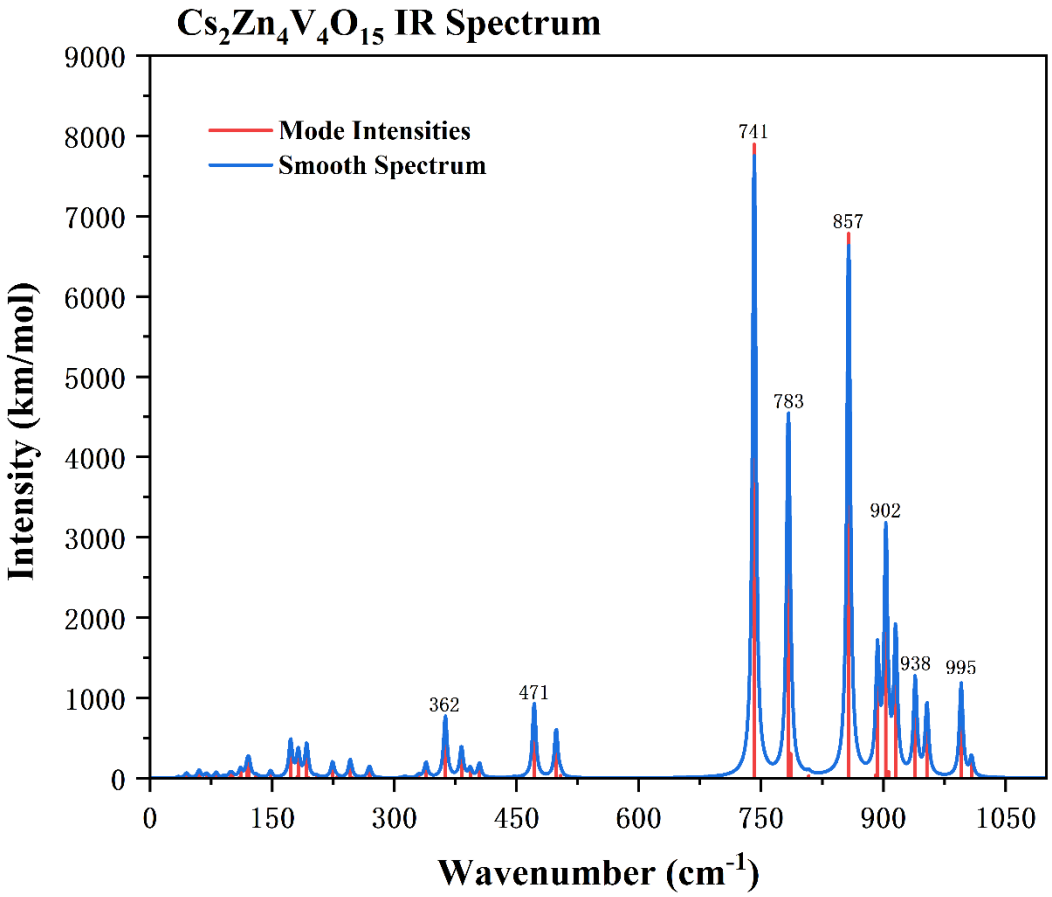

Figure S5. The obtained infrared spectrum of compound $Cs_2Zn_4V_4O_{15}$ obtained by DFT calculation.

References

1. N. E. Brese, M. Okeeffe, *Acta. crystallogr. B.* 1991, **47,** 192-197.
2. Y. Le Page, P. Strobel, *Inorg. Chem.* 1982, **21,** 620-623.
3. R. Hoppe, J. Kissel, *Z. Anorg. Allg. Chem.* 1989, **571,** 113-126.
4. J. Kissel, R. Hoppe, Z. *Anorg. Allg Chem.* 1990, **587,** 29-38.
5. G. J. Richard, *J. Mater. Chem.* 1992, **2,** 161-166.
6. R. áNandini Devi, *J. Chem. Soc. Dalton Trans.* 1998,**18,** 3013-3020.
7. L. Rghioui, L. El Ammari, L. Benerafa, M. Knidiri, A. Lorriaux, F. Wallart, H. Krautscheid, Can. *J. Anal. Sci. Spectros.* 1999, **44,** 89-96.
8. C. Wu, X. X. Jiang, L. Lin, Y. L. Hu, T. H. Wu, Z. S. Lin, Z. P. Huang, M. G. Humphrey, C. Zhang, *Angew. Chem. Int. Ed*. 2021, **133,** 22621-22627.
9. B. V. Slobodin; L. L. Surat, V. G. Zubkov, A. P. Tyutyunnik, I. F. Berger, M. V. Kuznetsov, L. A. Perelyaeva, I. R. Shein, A. L. Ivanovskii, B. V. Shulgin, V. I. Solomonov, G. Svensson, B. Forslund, M. J. Structural, *Phys. Rev. B.* 2005, **72,** 155205.
10. A. K. Paidi, R. N. Devi, K. Vidyasagar, *Dalton. Trans.* 2015, **44,** 17399-17408.
11. V. G. Zubkov, A. P. Tyutyunnik, I. F. Berger, L. L. Surat, B. V. Slobodin, *Neorg. Khim.* 2003, **48,** 2074-2079.
12. V. Hlukhyy, T. F. Faessler, *Angew. Chem. Int. Ed.* 2012, **51.** 4058-4065.
13. V. G. Zubkov, A. P. Tyutyunnik, N. V. Tarakina, I. F. Berger, L. L. Surat, B. V. Slobodin, A. N. Cherepanov, *Solid. State. sci.* 2009, **11,** 726-732.
14. F. C. Hawthorne, C. Calvo, *J. Solid. State. Chem.* 1977, **22,** 157-170.
15. T. M. Smith Pellizzeri, C. D. McMillen, Y. Wen, G. Chumanov, J. W. Eur. Kolis, *J. Inorg. Chem*. 2019, **2019,** 4538-4545.
16. K. Waltersson, *Acta. Crystallogr. B.* 1977, **33,** 784-789.
17. K. Waltersson, B. Forslund, *Acta. Crystallogr. B.* 1977, **33,** 789-793.
18. H. T. Evans Jr, *Inorg. Chem.* 1966, **5,** 967-977.
19. I. Duribreux, C. Dion, F. Abraham, M. Saadi, *J. Solid. State. Chem.* 1999, **146,** 258-265.
20. J. Yeon, A. S. Sefat, T. T. Tran, P. S. Halasyamani, H. C. zur Loye, *Inorg. chem.* 2013, **52,** 6179-6186.
21. Y. Wang, J. Liang, T. Wen, K. Li, Y. Wang, G. Li, F. Liao, J. Lin, *Solid. State. Chem.* 2012, **192,** 1-6.
22. K. Waltersson, B. Forslund, *Acta. Crystallogr. B.* 1977, **33,** 775-779.
23. V. G. Zubkov, A. P. Tyutyunnik, I. F. Berger, L. L. Surat, N. V. Tarakina, B. V. Slobodin, V. G. Bamburov, *Dokl. Akad .Nauk.* 2008, **421,** 506-510.
24. R. Gopal, C. Calvo, *Can. J. of Chem.* 1973, **51,** 1004-1009.
25. Y. Matsushima, A. Sato, M. Kitaura, H. Kominami, K. Hara, *J. Ceram. Soc. Jpn.* 2019, **127,** 627-635.
26. N. Guskos, A. Bezkrovnyi, J. Typek, N. Yu. Ryabova, A. Blonska-Tabero, M. Kurzawa, M. Maryniak, *J. Alloy. Compd.* 2005, **391,** 20-25.

27. M. Schindler, F. C. Hawthorne, *J. Solid. State. Chem*. 1999, **146,** 271-276.
28. M. Waburg, H. Müller-Buschbaum, *Monatsh. Chem.* 1986, **117,** 131-138.
29. M. Von Postel, H. Müller-Buschbaum, *Z. Anorg. Allg. Chem.* 1992, **615,** 97-100.
30. H. Müller-Buschbaum, M. von Postel, E *Z. Anorg. Allg. Chem.* 1992, **615,** 101-103.
31. C. Müller, H. Müller-Buschbaum, *J. Alloy. Compd.* 1993, **191,** 251-253.
32. E. V. Murashova, Yu. A. V. K. Velikodnyi, *Zh. Neorg. Khim*. 1989, **34,** 1388-1392.
33. A. Nakatsuka, Y. Ikuta, A. Yoshiasa, K. Iishi, *Mater. Res. Bull.* 2004, *39*, 949-956.
34. A. Bhim, W. Zhang, P. S. Halasyamani, J. Gopalakrishnan, S. Natarajan, *Inorg. Chem.* 2019, **58,** 8560-8569.
35. N. E. Lamsakhar, M. H. Hadouchi, M. Zriouil, A. Assani, M. Saadi, A. Lahmar, M. El Marssi, L. El Ammari, *Inorg. Chem. Commun.* 2019, **107,** 107472.
36. A. P. Tyutyunnik, V. G. Zubkov, L. L. Surat, B. V. Slobodin, G. Svensson, *Powder. diffr.* 2005, **20,** 189-192.
37. N. Wang, Z. He, M. Cui, W. Guo, S. Zhang, M. Yang, *Cryst. Growth Des.* 2015, **15,** 1619-1624.
38. H. Yu, J. Young, H. Wu, W. Zhang, J. M. Rondinelli, P. S. Halasyamani, *J. Am. Chem. Soc.* 2016, **138,** 4984-4989.
39. A. P. Malakho, O. L. Vorontsova, V. A. Morozov, S. Yu. Stefanovich, B. I. Lazoryak, *Zh. Neorg. Khim.* 2004, **49,** 165-173.
40. T. Hasegawa, Y. Abe, A. Koizumi, T. Ueda, K. Toda, M. Sato, *Inorg. Chem.* 2018, **57,** 857-866.
41. N. E. H. Lamsakhar, M. Zriouil, A. Assani, M. Saadi, L. El Ammari, *Acta. Crystallogr. E.* 2018, **74,** 1155-1158.
42. D. G. Chen, W. D. Cheng, D. S. Wu, H. Zhang, Y. C. Zhang, Y. J. Gong, Z. G. Kan, *Solid. State. Chem.* 2004, **177,** 3927-3933.
43. R. Madhuri, S. Ganesanpotti, *J. Am. Ceram.* Soc. 2020, **103,** 3157-3167.
44. M. Zheng, P. Lv, D. Chen, F. Yan, F. Huang, *J. Struc. Chem*. 2013, *32*, 106-112.
45. L. K. Bharat, K. G. Krishna, J. S. Yu, J. Alloy. Compd. 2017, **699,** 756-762.
46. X. Shan, S. Kim, A. M. Abeykoon, G. Kwon, D. Olds, X. Teng, ACS. Appl. Mater. Interfaces. 2020, **12,** 54627-54636.
47. A. Bhatia, J. Xu, J. P. Pereira-Ramos, G. Rousse, R. Baddour-Hadjean, *Chem. Mater.* 2021, **34,** 1203-1212.
48. X. Wang, D. Vander Griend, C. L. A. Stern, K. R. Poeppelmeier, *J. Alloy. Compd.* 2000, **298,** 119-124.
49. S. J. Hong, J. Li, M. A. Subramanian, *Acta. Crystallogr. E.* 2021, **77,** 588-591.
50. V. D. Zhuravlev, A. P. Tyutyunnik, A. Y. Chufarov, N. I. Lobachevskaya, A.

A. Velikodnyi, *Powder. Diffr.* 2018, **33,** 216-224.
51. E. V. Murashova, Yu. A. Velikodnyi, V. K. Trunov, *Kristallografiya.* 1991, **36,** 617-621.
52. D. Capsoni, M. Bini, V. Massarotti, P. Mustarelli, F. Belotti, P. Galinetto, *J. Phy. Chem.* B. 2006, **110,** 5409-5415.
53. D. J. Lloyd, J. Galy, *Struct. Commun.* 1973, **2,** 209-211.