Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Nonlinear Optical and Self-activated Luminescent Properties of $A_2W_3O_{10}$ (A = Rb and Cs)

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Table S1 Crystal Data and Structure Refinements for $Rb_2W_3O_{10}$ and $Cs_2W_3O_{10}$.

Empirical Formula	$Rb_2W_3O_{10}$	$Cs_2W_3O_{10}$
Crystal system	Tetragonal	Tetragonal
space group	$I\bar{4}$	$I\bar{4}$
a (Å)	15.9516(9)	16.0980(9)
c (Å)	10.0565(11)	10.1703(11)
volume (Å^3)	2558.9(3)	2635.6(4)
Z	120/11	120/11
density (calcd) (mg/cm^3)	4.581	4.926
abs coeff (mm^{-1})	34.493	31.594
cryst size (mm^3)	0.107×0.139 × 0.167	0.130×0.133×0.134
the range for data collection (deg)	2.39 to 27.45	2.37 to 24.98
index ranges	$-14 \le h \le 20$, $-20 \le k \le 18$, $-13 \le l \le 12$	$-17 \le h \le 19$, $-19 \le k \le 19$, $-12 \le l \le 9$
reflns collected /unique	7864 / 2886 [R(int)=0.0691]	6688 / 2305 [R(int) = 0.0515]
completeness	99.9 %	99.8 %
data/restraints/param	2886 / 31 / 211	2306 / 31 / 211
GOF on F^2	1.042	1.089
final R indices [$Fo^2>2\sigma(Fo^2)$][a]	R_1 = 0.0488, wR_2 = 0.1132	R_1 = 0.0466, wR_2=0.1150
R indices (all data)[a]	R_1 = 0.0534, wR_2=0.1169	R_1 = 0.484, wR_2= 0.1167
Absolute structure parameter	0.00	0.00
extinction coeff	0.00057(4)	0.0000(13)
largest diff peak and hole (e/Å^3)	6.972 and -3.970	11.759 and -2.948

Table S2 Atomic coordinates and equivalent isotropic displacement parameters for $Rb_2W_3O_{10}$ and $Cs_2W_3O_{10}$.

Atoms	*x*	*y*	*z*	U_{eq}(Å^2)	OCC
W(1)	0.9620(1)	0.3914(1)	0.1164(1)	0.008(1)	1
W(2)	0.7381(1)	0.5156(1)	0.6650(1)	0.013(1)	1
W(3)	0.8689(1)	0.1828(1)	0.1465(1)	0.012(1)	1
W(4)	0.8520(1)	0.7208(1)	0.5873(1)	0.012(1)	1
W(5)	0.9010(6)	0.0500(5)	0.3764(10)	0.008(2)	0.092
Rb(1)	1.0000	0	0.5000	0.097(4)	0.908
Rb(2)	1.0000	0.5000	0.7500	0.087(4)	1
Rb(3)	0.9102(2)	0.2936(3)	0.4941(4)	0.050(1)	1
Rb(4)	0.5000	0.5000	0.5000	0.080(4)	1
Rb(5)	0.1149(2)	0.2159(2)	0.2176(3)	0.026(1)	1
O(1)	0.9079(10)	0.2966(9)	0.1876(14)	0.009(3)	1
O(2)	0.0144(9)	0.3347(9)	0.9893(16)	0.006(3)	1
O(3)	0.7997(9)	0.6101(11)	0.6894(14)	0.009(3)	1
O(4)	0.8630(9)	0.4107(8)	0.0116(15)	0.002(3)	1
O(5)	0.6853(10)	0.5618(11)	0.5064(19)	0.017(4)	1
O(6)	0.7581(11)	0.7139(9)	0.4821(18)	0.014(4)	1
O(7)	0.0429(9)	0.3924(9)	0.2429(16)	0.007(3)	1
O(8)	0.8107(11)	0.0903(10)	0.0841(16)	0.016(4)	1
O(9)	0.7985(10)	0.4448(10)	0.7748(15)	0.013(4)	1
O(10)	1.0000	0.5000	0.0560(20)	0.007(4)	1
O(11)	0.9002(12)	0.8097(11)	0.5130(20)	0.024(4)	1
O(12)	0.7813(10)	0.2058(11)	0.2735(16)	0.013(3)	1
O(13)	0.9385(13)	0.1328(11)	0.2550(20)	0.025(4)	1
O(14)	0.6503(11)	0.5350(13)	0.7700(20)	0.023(4)	1
O(15)	0.9030(30)	0.972(110)	0.5060(160)	0.030(50)	0.092
O(16)	1.0000	0	0.6690(20)	0.020(60)	0.092

Atoms	*x*	*y*	*z*	U_{eq}(Å^2)	OCC
W(1)	0.9588(1)	0.3938(1)	0.1191(1)	0.008(1)	1
W(2)	0.7408(1)	0.5111(1)	0.6559(1)	0.014(1)	1
W(3)	0.8634(1)	0.1868(1)	0.1414(1)	0.012(1)	1
W(4)	0.8523(1)	0.7163(1)	0.5977(1)	0.013(1)	1
W(5)	0.9002(6)	0.0499(6)	0.3748(11)	0.000(2)	0.092
Cs(1)	1.0000	0	0.5000	0.063(2)	0.908
Cs(2)	1.0000	0.5000	0.7500	0.035(1)	1
Cs(3)	0.9043(1)	0.2965(1)	0.4987(2)	0.019(1)	1
Cs(4)	0.5000	0.5000	0.5000	0.028(1)	1
Cs(5)	0.1114(1)	0.2137(1)	0.2254(2)	0.023(1)	1
O(1)	0.9029(12)	0.3001(11)	0.1820(17)	0.013(4)	1
O(2)	0.0121(11)	0.3355(12)	0.9950(20)	0.019(5)	1
O(3)	0.8003(11)	0.6063(12)	0.6859(18)	0.016(4)	1
O(4)	0.8636(13)	0.4100(11)	0.0010(20)	0.019(5)	1
O(5)	0.6889(10)	0.5639(11)	0.5030(20)	0.013(4)	1
O(6)	0.7625(13)	0.7123(10)	0.4890(20)	0.019(5)	1
O(7)	0.0382(11)	0.3903(10)	0.2485(18)	0.006(4)	1
O(8)	0.8079(10)	0.0945(9)	0.0765(16)	0.006(4)	1
O(9)	0.8027(10)	0.4410(9)	0.7636(18)	0.006(4)	1
O(10)	1.0000	0.5000	0.0590(20)	0.000(4)	1
O(11)	0.9007(10)	0.8038(11)	0.5370(20)	0.016(5)	1
O(12)	0.7724(11)	0.2068(10)	0.2645(17)	0.007(4)	1
O(13)	0.9262(13)	0.1376(11)	0.2530(20)	0.019(5)	1
O(14)	0.6563(12)	0.5249(11)	0.7600(20)	0.015(4)	1
O(15)	0.9040(20)	0.974(70)	0.5050(110)	0.000(30)	0.092
O(16)	1.0000	0	0.6670(20)	0.000(50)	0.092