Supporting information

Photoluminescent and photovoltaic properties observed in a zinc borate $Zn_2(OH)BO_3$

Zhen-Tao Yu, Jin-Jie Xu, Yu-Sheng Jiang, Zhan Shi, Ying Guo, De-Jun Wang and Jie-Sheng Chen*

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130023, P. R. China. Fax: (+86) 431 5671974; E-mail: chemcj@mail.jlu.edu.cn.

Table S1. Crystal data and structure refinement for $Zn_2(OH)BO_3$.

Empirical formula	$Zn_2(OH)BO_3$
Formula weight	206.56
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 5.7222(5) Å α = 90°
	b = 4.9314(3) Å β = 98.786(4)°
	c = 6.8872(4) Å γ = 90°
Volume	192.07(2) $Å^3$
Z	2
Calculated density	3.572 Mg/m^3
Absorption coefficient	12.347 mm^{-1}
F(000)	196
Crystal size	0.20 x 0.03 x 0.03 mm
Theta range for data collection	2.99 to 23.21°
Limiting indices	$-3\le h\le 6$, $-5\le k\le 5$, $-7\le l\le 7$
Reflections collected / unique	945 / 555 [R(int) = 0.0339]
Completeness to theta =	23.21 99.7 %
Max. and min. transmission	0.7083 and 0.1915
Refinement method	Full-matrix least-squares on F^2
Data / parameters	555 / 64
Goodness-of-fit on F^2	1.108
Final R indices [I>2sigma(I)]	R1 = 0.0287, wR2 = 0.0714
Absolute structure parameter	-0.06(4)
Largest diff. peak and hole	0.588 and –0.939 e. $Å^{-3}$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Zn_2(OH)BO_3$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	*U*(eq)[a]
Zn(1)	4436(1)	9369(1)	3552(1)	13(1)
Zn(2)	-723(1)	9542(2)	1276(1)	13(1)
O(1)	1567(7)	11630(9)	3041(7)	14(1)
O(2)	3456(8)	5737(9)	4168(7)	16(1)
O(3)	5860(6)	9563(14)	1146(6)	18(1)
O(4)	339(8)	5743(9)	1431(7)	15(1)
B(1)	1752(9)	4460(20)	2907(9)	11(1)

Table S3. Bond lengths [Å] and angles [º] for $Zn_2(OH)BO_3$[a].

Zn(1)-O(2)	1.943(5)	Zn(2)-O(1)	1.942(5)
Zn(1)-O(2)#1	1.949(5)	Zn(2)-O(3)#2	1.943(4)
Zn(1)-O(3)	1.957(4)	Zn(2)-O(4)	1.968(4)
Zn(1)-O(1)	1.971(4)	Zn(2)-O(4)#3	2.000(4)
Zn(1)-Zn(2)	3.1254(8)		
B(1)-O(2)	1.359(9)	B(1)-O(1)#8	1.402(12)
B(1)-O(4)	1.356(9)		
O(2)-Zn(1)-O(2)#1	107.87(15)	O(1)-Zn(2)-O(3)#2	127.2(2)
O(2)-Zn(1)-O(3)	113.7(2)	O(1)-Zn(2)-O(4)	107.30(18)
O(2)#1-Zn(1)-O(3)	112.26(19)	O(3)#2-Zn(2)-O(4)	107.9(2)
O(2)-Zn(1)-O(1)	107.45(19)	O(1)-Zn(2)-O(4)#3	105.49(19)
O(2)#1-Zn(1)-O(1)	110.1(2)	O(3)#2-Zn(2)-O(4)#3	102.04(18)
O(3)-Zn(1)-O(1)	105.3(2)	O(4)-Zn(2)-O(4)#3	104.82(15)
O(2)-Zn(1)-Zn(2)	81.53(14)	O(1)-Zn(2)-Zn(1)	37.32(13)
O(2)#1-Zn(1)-Zn(2)	144.66(14)	O(3)#2-Zn(2)-Zn(1)	152.85(12)
O(3)-Zn(1)-Zn(2)	93.30(11)	O(4)-Zn(2)-Zn(1)	71.71(13)
O(1)-Zn(1)-Zn(2)	36.66(14)	O(4)#3-Zn(2)-Zn(1)	104.23(13)
O(4)-B(1)-O(2)	123.3(9)	O(4)-B(1)-O(1)#8	118.2(6)
O(2)-B(1)-O(1)#8	118.3(6)		

[a] Symmetry transformations used to generate equivalent atoms:

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

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Zn_2(OH)BO_3$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U11+ ... + 2hkabU12]$.

	U11	U22	U33	U23	U13	U12
Zn(1)	17(1)	5(1)	16(1)	0(1)	-2(1)	0(1)
Zn(2)	16(1)	5(1)	16(1)	-1(1)	-1(1)	-1(1)
O(1)	21(2)	1(2)	19(2)	-1(2)	-3(2)	1(2)
O(2)	23(2)	6(2)	19(2)	2(2)	-2(2)	1(2)
O(3)	17(2)	17(2)	20(2)	2(3)	3(2)	-1(2)
O(4)	20(2)	8(2)	14(2)	-4(2)	0(2)	1(2)
B(1)	10(3)	11(3)	14(3)	-5(5)	3(3)	-1(4)

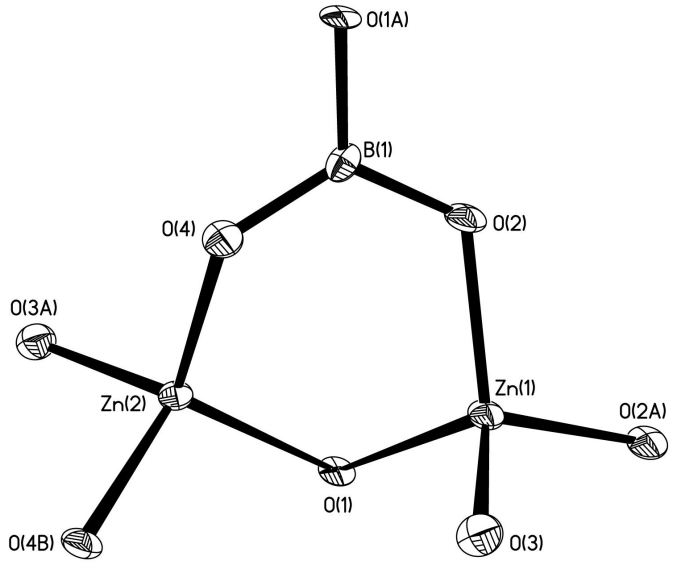

Figure S1. ORTEP plot of $Zn_2(OH)BO_3$ (50% probability).

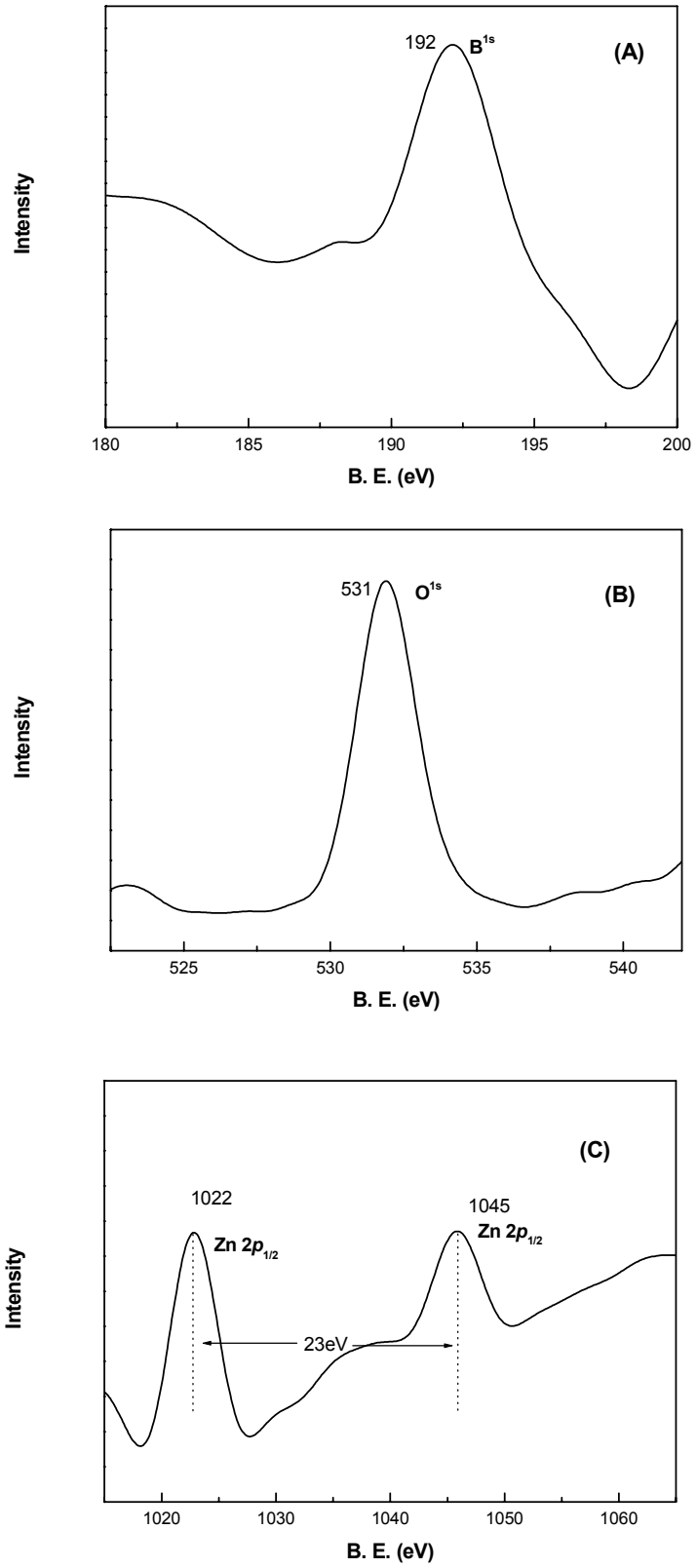

Figure S2. XPS spectra for (A) B 1s, (B) O 1s and (C) Zn 2p in $Zn_2(OH)BO_3$.

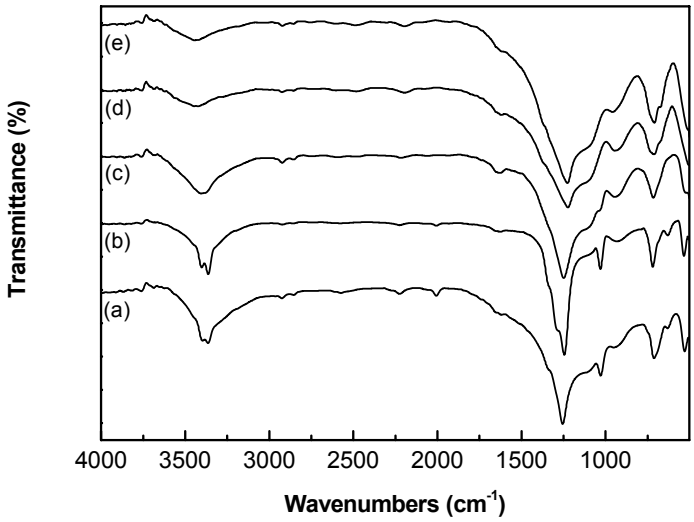

Figure S3. Room temperature IR spectra for (a) the as-prepared $Zn_2(OH)BO_3$ and the samples calcined at (b) 400, (c) 500, (d) 560 and (e) 650 °C for 3.5 h.

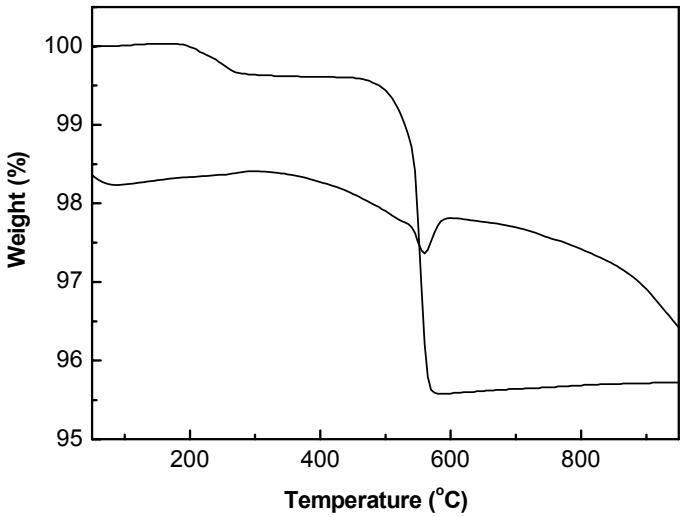

Figure S4. TG and DTA curves of $Zn_2(OH)BO_3$.