Electronic Supplementary Information

$Mg(H_2O)_6B_4O_5(OH)_4(H_2O)_3$: A new hydrated borate with a short DUV cutoff edge

Ya Wang,[†a,b] Jian Han,[†a] Fengjiao Guo,[†a,b] Shichao Cheng,[a] Zhihua Yang[a] and Shilie Pan[*a]

[a] CAS Key Laboratory of Functional Materials and Devices for Special Environments; Xinjiang Technical Institute of Physics & Chemistry, CAS; Xinjiang Key Laboratory of Electronic Information Materials and Devices, 40-1 South Beijing Road, Urumqi 830011, China.

[b] Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China.

[†] These authors contributed equally to this work.

* Corresponding author: slpan@ms.xjb.ac.cn.

Table S1. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $Mg(H_2O)_6B_4O_5(OH)_4(H_2O)_3$.

Atom	x	y	z	U(eq)
Mg(1)	7378(1)	7610(1)	6644(1)	25(1)
B(1)	6712(2)	2777(2)	9837(2)	20(1)
B(2)	8427(2)	4066(2)	9979(2)	17(1)
B(3)	8474(2)	3041(2)	8254(2)	21(1)
B(4)	6638(2)	4049(2)	8190(2)	19(1)
O(1)	8396(2)	9184(2)	7348(2)	35(1)
O(2)	8505(2)	7177(2)	5881(2)	40(1)
O(3)	8396(2)	6517(2)	8054(2)	38(1)
O(4)	6195(2)	6157(2)	5815(2)	28(1)
O(5)	6327(2)	7993(2)	7502(2)	37(1)
O(6)	6398(2)	8748(2)	5212(2)	45(1)
O(7)	6138(2)	1988(2)	10288(2)	32(1)
O(8)	7861(1)	3167(1)	10494(1)	21(1)
O(9)	6089(1)	3137(2)	8712(1)	23(1)
O(10)	7494(1)	4832(1)	9115(1)	18(1)
O(11)	5714(1)	4744(2)	7282(1)	24(1)
O(12)	9297(1)	4772(2)	10939(1)	22(1)
O(13)	9073(1)	3351(1)	9397(1)	21(1)
O(14)	7287(1)	3329(2)	7616(1)	23(1)
O(15)	9110(2)	2403(2)	7772(2)	32(1)
O(16)	4097(2)	5894(2)	8121(1)	62(1)
O(17)	2673(1)	4803(2)	5595(1)	55(1)
O(18)	327(1)	5971(2)	4490(1)	50(1)
H(1A)	8640(20)	9590(20)	6930(20)	42
H(1B)	8980(20)	9120(30)	7997(18)	42
H(2A)	9262(16)	7180(30)	6310(20)	48
H(2B)	8320(30)	6680(20)	5330(20)	48
H(3A)	9055(18)	6200(30)	8230(30)	45
H(3B)	8090(20)	6020(20)	8370(20)	45
H(4A)	5486(16)	6380(20)	5350(20)	33
H(4B)	6120(20)	5680(20)	6310(20)	33
H(5A)	5540(16)	8020(30)	7140(20)	44
H(5B)	6520(30)	8460(20)	8070(20)	44
H(6A)	5708(18)	8700(30)	4700(20)	55
H(6B)	6710(30)	9160(30)	4850(30)	55
H(7)	6550(20)	1820(30)	10990(16)	38
H(11)	5250(20)	5140(20)	7500(20)	29
H(12)	9580(20)	5344(19)	10710(20)	26
H(15)	8730(20)	2280(30)	7053(16)	39

H(16A)	3600	5360	8160	93
H(16B)	3716	6541	7763	93
H(17A)	3012	5286	6175	83
H(17B)	3095	4771	5207	83
H(18A)	293	6692	4759	75
H(18B)	1061	5742	4740	75

Table S2. Bond distances (Å) and angles (deg.) for $Mg(H_2O)_6B_4O_5(OH)_4(H_2O)_3$.

Mg(1)-O(2)	2.041(2)	O(5)-Mg(1)-O(6)	95.06(9)
Mg(1)-O(5)	2.043(2)	O(3)-Mg(1)-O(6)	178.01(8)
Mg(1)-O(3)	2.056(2)	O(16)-H(16B)	0.8501
Mg(1)-O(1)	2.058(2)	O(17)-H(17A)	0.8500
Mg(1)-O(4)	2.078(2)	O(17)-H(17B)	0.8501
Mg(1)-O(6)	2.092(2)	O(18)-H(18A)	0.8501
B(1)-O(7)	1.366(3)	O(18)-H(18B)	0.8501
B(1)-O(8)	1.360(3)	O(2)-Mg(1)-O(5)	176.40(9)
B(1)-O(9)	1.359(3)	O(2)-Mg(1)-O(3)	90.18(9)
B(2)-O(8)	1.485(3)	O(5)-Mg(1)-O(3)	86.29(9)
B(2)-O(10)	1.454(3)	O(2)-Mg(1)-O(1)	89.20(9)
B(2)-O(12)	1.445(3)	O(5)-Mg(1)-O(1)	90.28(9)
B(2)-O(13)	1.498(3)	O(3)-Mg(1)-O(1)	93.10(9)
B(3)-O(13)	1.360(3)	O(2)-Mg(1)-O(4)	93.16(8)
B(3)-O(14)	1.364(3)	O(5)-Mg(1)-O(4)	87.74(8)
B(3)-O(15)	1.358(3)	O(3)-Mg(1)-O(4)	93.02(8)
B(4)-O(9)	1.487(3)	O(1)-Mg(1)-O(4)	173.43(9)
B(4)-O(10)	1.462(3)	O(2)-Mg(1)-O(6)	88.45(10)
B(4)-O(11)	1.433(3)	O(8)-B(1)-O(7)	120.8(2)
B(4)-O(14)	1.495(3)	O(12)-B(2)-O(10)	113.88(19)
O(1)-H(1A)	0.831(17)	O(12)-B(2)-O(8)	106.26(19)
O(1)-H(1B)	0.834(17)	O(10)-B(2)-O(8)	109.50(18)
O(2)-H(2A)	0.854(17)	O(12)-B(2)-O(13)	109.18(18)
O(2)-H(2B)	0.837(17)	O(10)-B(2)-O(13)	108.88(18)
O(3)-H(3A)	0.813(17)	O(8)-B(2)-O(13)	109.02(18)
O(3)-H(3B)	0.851(17)	O(15)-B(3)-O(13)	116.7(2)
O(4)-H(4A)	0.852(16)	O(15)-B(3)-O(14)	120.9(2)
O(4)-H(4B)	0.846(17)	O(13)-B(3)-O(14)	122.5(2)
O(5)-H(5A)	0.880(17)	O(11)-B(4)-O(10)	113.8(2)
O(5)-H(5B)	0.824(17)	O(11)-B(4)-O(9)	110.33(18)
O(6)-H(6A)	0.820(17)	O(10)-B(4)-O(9)	108.75(19)
O(6)-H(6B)	0.835(18)	O(11)-B(4)-O(14)	105.94(19)
O(7)-H(7)	0.835(17)	O(10)-B(4)-O(14)	109.82(18)
O(11)-H(11)	0.831(16)	O(9)-B(4)-O(14)	108.06(19)
O(12)-H(12)	0.816(16)	O(9)-B(1)-O(8)	122.1(2)

O(15)-H(15)	0.842(17)	O(9)-B(1)-O(7)	117.1(2)
O(16)-H(16A)	0.8501		

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

Table S3. Hydrated borates containing Mg atoms.

Compounds	**Anionic units**	**Dimensionality**	**Mg/B**
$Mg_3B_{11}O_{15}(OH)_9$	$B_{11}O_{16}(OH)_9$	3 D	0.27
$MgB_{12}O_{19}(H_2O)_5$	$B_6O_7(OH)_5$	2 D	0.08
$MgB_6O_9(OH)_2(H_2O)_4$	$B_6O_{11}(OH)_2$	2 D	0.17
$MgB_6O_7(OH)_6(H_2O)_3$	$B_6O_7(OH)_6$	0 D	0.17
$MgB_6O_7(OH)_6(H_2O)_2$	$B_6O_7(OH)_6$	0 D	0.17
$Mg_2[B_6O_7(OH)_6]_2(H_2O)_9$	$B_6O_{10}(OH)_3$	0 D	0.17
$(MgO)(B_2O_3)_3(H_2O)_5$	$B_6O_7(OH)_6$	0 D	0.17
$MgO(B_2O_3)_3(H_2O)_6$	$B_6O_7(OH)_6$	0 D	0.17
$MgO(B_2O_3)_3(H_2O)_7$	$B_6O_7(OH)_6$	0 D	0.17
$MgB_4O_4(OH)_6(H_2O)_6$	$B_4O_4(OH)_6$	0 D	0.25
$Mg(H_2O)_5B_4O_5(OH)_4(H_2O)_2$	$B_4O_5(OH)_4$	0 D	0.25
$MgB_3O_3(OH)_5(H_2O)_5$	$B_3O_3(OH)_5$	0 D	0.33
$Mg(H_2O)_4B_3O_3(OH)_5(H_2O)$	$B_3O_3(OH)_5$	0 D	0.33
$Mg_2B_6O_{11}(H_2O)_{15}$	$B_3O_3(OH)_5$	0 D	0.33
$MgB_2O(OH)_6$	$B_2O(OH)_6$	0 D	0.5
$MgBO_2(OH)$	$B_2O_4(OH)$	0 D	1
$Mg_3(BO_3)(OH)_3$	BO_3	0 D	3
$Mg_5O(OH)_5(BO_3)(H_2O)_{1.4}$	BO_3	0 D	5

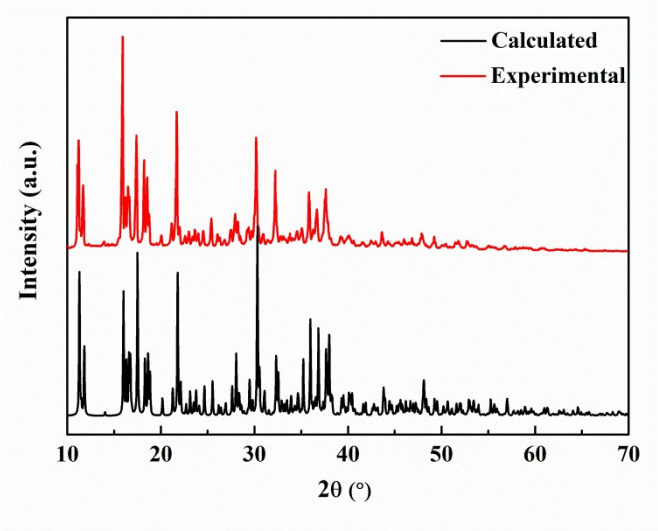

Fig. S1 The XRD patterns of $Mg(H_2O)_6B_4O_5(OH)_4(H_2O)_3$.

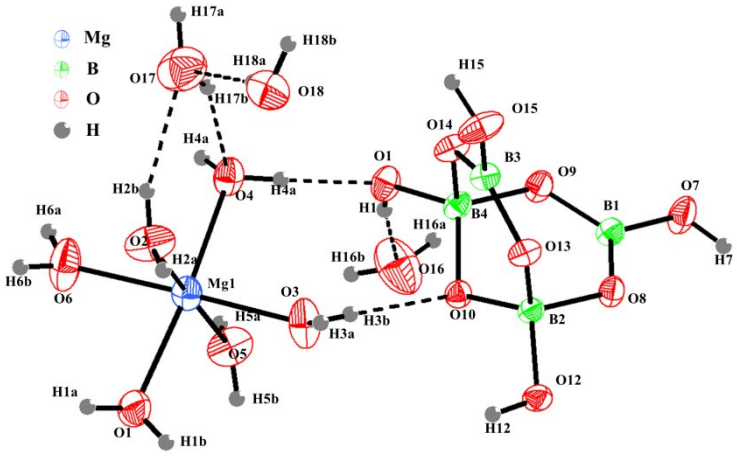

Fig. S2 The asymmetric unit of $Mg(H_2O)_6B_4O_5(OH)_4(H_2O)_3$.

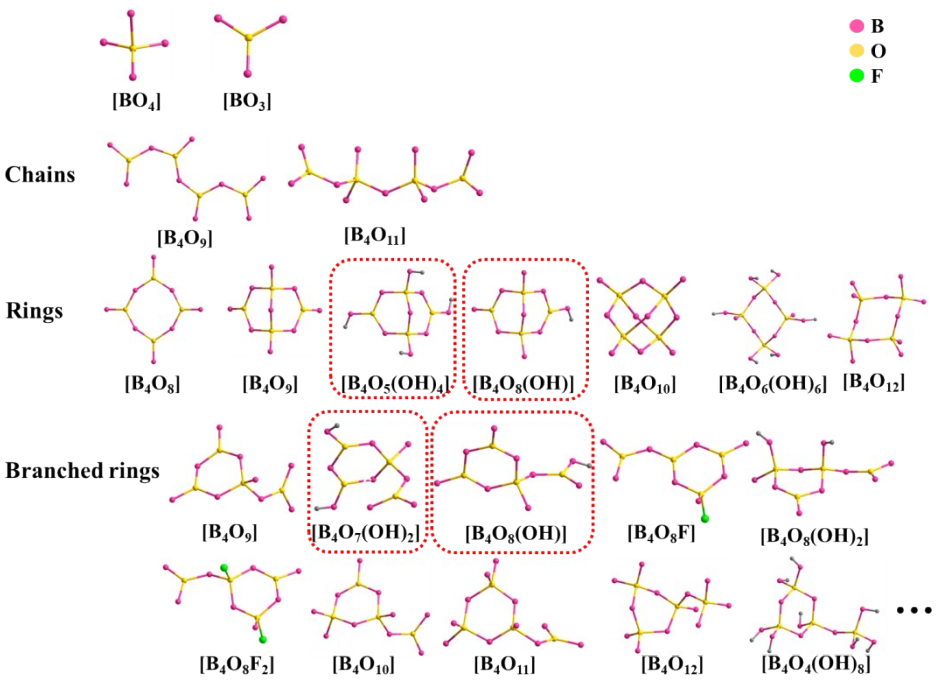

Fig. S3 The types of four-polymeric FBBs.

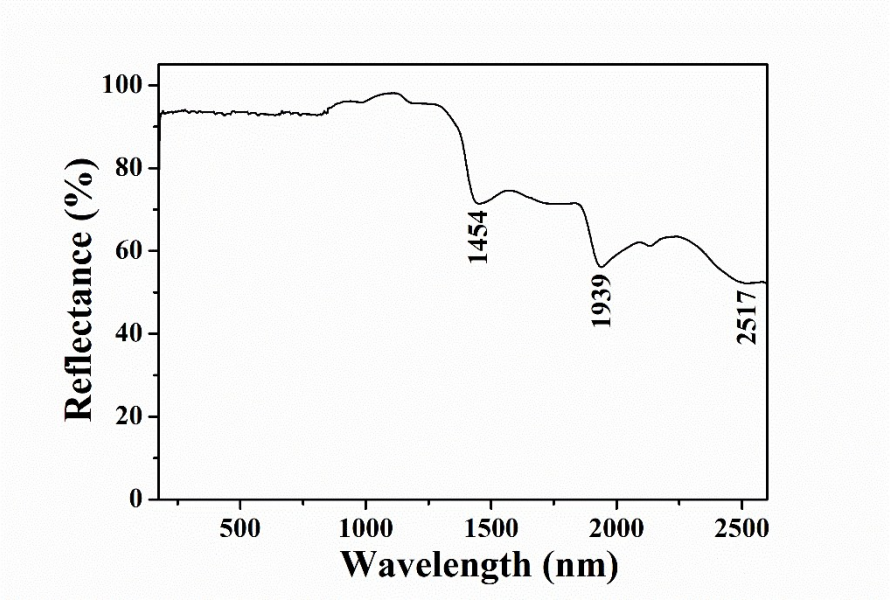

Fig. S4 The UV-Vis-NIR spectrum of $Mg(H_2O)_6B_4O_5(OH)_4(H_2O)_3$.