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Supporting Information

$Zn_4B_3O_9C_2H_8N_2$: An organic-inorganic hybrid borate with novel graphene-like layer

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Table S1. Selected bond lengths and bond angles for $Zn_4B_3O_9C_2H_8N_2$[a]

Zn(1)-O(4)	1.922(8)	B(2)-O(4)	1.3391(11)
Zn(1)-O(5)	1.935(7)	B(1)-O(2)#1	1.380(8)
Zn(1)-O(3)#1	1.951(4)	B(1)-O(3)	1.367(7)
Zn(1)-O(2)	1.952(4)	B(2)-O(5)	1.3398(11)
Zn(1)-O(3)	1.968(4)	C(1)-C(1)#5	1.460(13)
Zn(2)-O(2)	1.939(4)	C(1)-N(1)	1.507(9)
Zn(2)-O(1)#2	1.944(4)	B(1)#1-O(1)	1.361(7)
Zn(2)-O(1)	1.956(4)	Zn(2)#6-O(1)	1.944(4)
Zn(2)-N(1)	2.019(5)	B(1)#3-O(2)	1.380(8)
B(2)-O(6)	1.3385(11)	Zn(1)#3-O(3)	1.951(4)
O(1)#3-B(1)-O(3)	120.2(6)	O(6)-B(2)-O(5)	124.4(6)
O(1)#3-B(1)-O(2)#1	119.6(5)	O(6)#4-B(2)-O(4)	125.1(6)
O(3)-B(1)-O(2)#1	120.2(5)	O(6)-B(2)-O(4)#4	125.1(6)
O(4)#4-B(2)-O(5)	110.2(5)	O(6)#4-B(2)-O(5)#4	124.4(6)
O(2)-Zn(2)-O(1)#2	106.46(16)	O(4)-B(2)-O(5)#4	110.2(5)
O(2)-Zn(2)-O(1)	106.42(17)	O(3)#1-Zn(1)-O(3)	105.28(13)
O(1)#2-Zn(2)-O(1)	105.96(12)	O(2)-Zn(1)-O(3)	104.41(17)
O(5)-Zn(1)-O(3)#1	104.6(3)	O(2)-Zn(2)-N(1)	115.37(19)
O(5)-Zn(1)-O(2)	102.21(18)	O(1)#2-Zn(2)-N(1)	116.11(19)
O(3)#1-Zn(1)-O(2)	105.55(18)	O(1)-Zn(2)-N(1)	105.73(18)
O(4)-Zn(1)-O(3)#1	114.1(3)		

[a]Symmetry transformations used to generate equivalent atoms:

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

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

#5 -x+1,-y+2,-z+2 #6 -x+2,-y+2,-z+1

Table S2. Anisotropic displacement parameters for $Zn_4B_3O_9C_2H_8N_2$

Atom	U11	U22	U33	U23	U13	U12
Zn(1)	13(1)	12(1)	24(1)	0(1)	4(1)	0(1)
Zn(2)	12(1)	11(1)	27(1)	1(1)	4(1)	0(1)
B(1)	11(3)	8(4)	30(3)	-2(3)	1(3)	-6(3)
B(2)	15(2)	15(2)	16(2)	0(1)	2(1)	1(1)
C(1)	60(5)	36(5)	30(4)	1(3)	0(4)	8(4)
N(1)	22(3)	31(3)	26(3)	-1(2)	8(2)	-2(2)
O(1)	13(2)	9(2)	35(2)	-2(2)	4(2)	-2(2)
O(2)	12(2)	14(2)	41(2)	2(2)	10(2)	2(2)
O(3)	11(2)	13(2)	72(3)	-10(2)	-1(2)	4(2)
O(4)	33(5)	27(6)	35(5)	-3(4)	3(4)	-3(4)
O(5)	26(5)	33(6)	35(5)	5(4)	4(4)	4(4)
O(6)	82(9)	22(6)	62(8)	-11(5)	5(7)	-1(6)

Table S3. Hydrogen Bond (Å) for $Zn_4B_3O_9C_2H_8N_2$[b]

	D-H	H-A	D-A	D-H-A
N(1)-H(3)-O(4)[a]	0.93	2.08	3.009(10)	171
N(1)-H(3)-O(6)[a]	0.93	1.97	2.826(10)	152
N(1)-H(4)-O(6)[b]	0.92	1.99	2.866(10)	160
N(1)-H(4)-O(5)[c]	0.92	2.25	3.107(9)	156

[b]Symmetry Codes: (a)1-x, 1/2+y, 3/2-z (b)1-x, -1/2+y, 3/2-z (c)x, 3/2-y, -1/2+z

Figure S1 The crystal photograph of $Zn_4B_3O_9C_2H_8N_2$

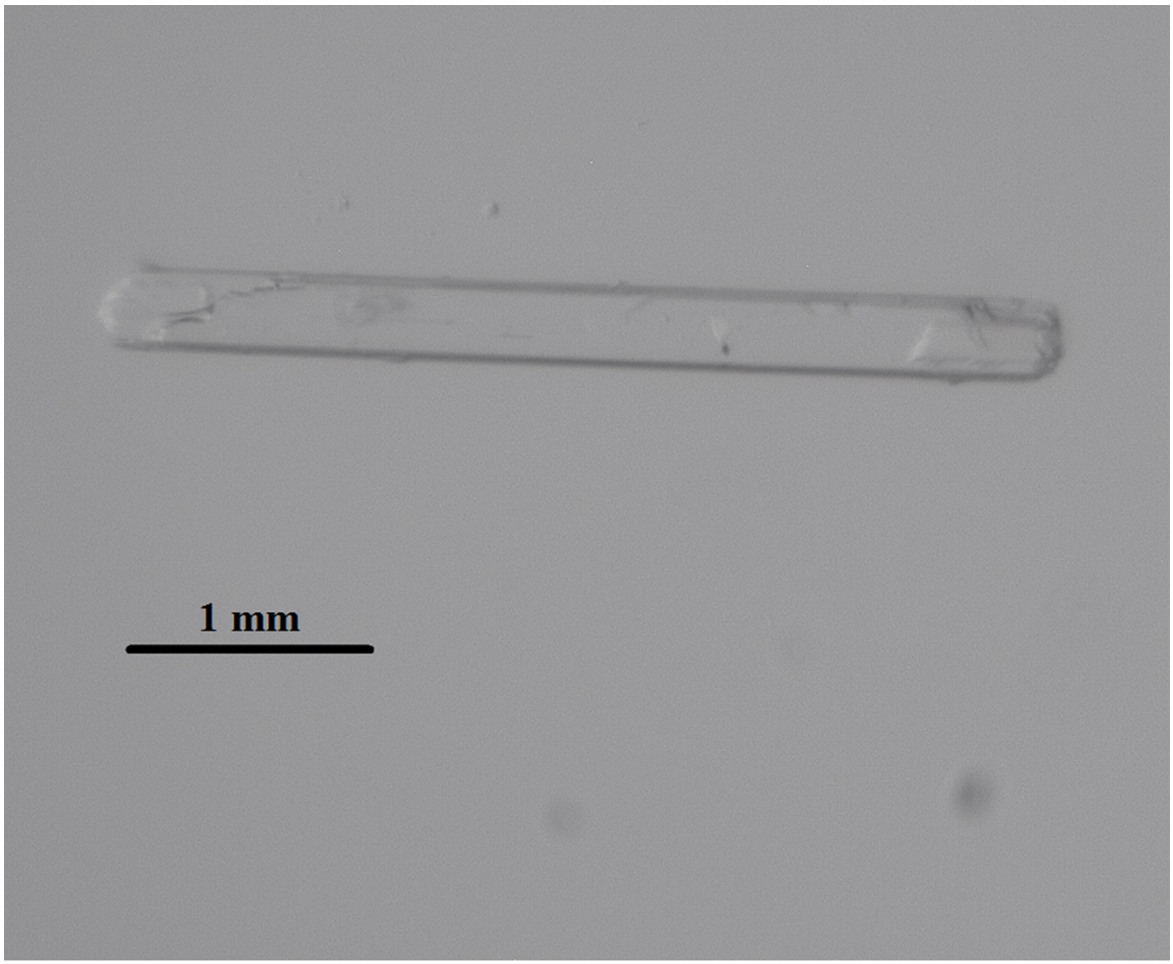

Figure S2 IR spectrum of $Zn_4B_3O_9C_2H_8N_2$