Electronic Supplementary Information for:

$NH_4B_{11}O_{16}(OH)_2$: A New Ammonium Borate with Wavy-Shaped Polycyclic $^{2}_{\infty}[B_{11}O_{16}(OH)_2]$ Layers

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Table S1. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$) and bond valence sum (BVS) calculations for $NH_4B_{11}O_{16}(OH)_2$. *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atoms	*x*	*y*	*z*	*U*(eq)	BVS
N(1)	5000	7926(4)	7500	37(1)	
B(1)	2791(2)	10224(3)	10076(3)	24(1)	2.8
B(2)	1432(2)	9336(4)	10681(3)	25(1)	3.1
B(3)	2252(2)	11240(3)	11731(3)	21(1)	3.0
B(4)	4054(2)	10913(3)	8975(3)	21(1)	3.1
B(5)	266(2)	7591(3)	9563(3)	22(1)	3.1
B(6)	5000	11488(5)	7500	20(1)	3.1
O(1) $_{\text{hydroxyl}}$	2347(1)	12239(2)	12569(2)	30(1)	1.1[a]
O(2)	2881(1)	11213(2)	10961(2)	24(1)	2.0
O(3)	1534(1)	10294(2)	11587(2)	28(1)	2.0
O(4)	2073(1)	9278(2)	9946(2)	30(1)	1.8
O(5)	3362(1)	10121(2)	9273(2)	28(1)	2.1
O(6)	4479(1)	11920(2)	9790(2)	26(1)	2.0
O(7)	4324(1)	10635(2)	7929(2)	22(1)	1.9
O(8)	663(1)	8496(2)	10504(2)	26(1)	2.1
O(9)	578(1)	7338(2)	8544(2)	23(1)	1.9
H(1)	1957	12138	12994	44	
H(2)	4762	7340	8032	150(20)	
H(3)	5093	8579	8016	270(40)	

[a] bond valence sum of O1 without hydrogen coordinates.

Table S2. Selected bond lengths (Å) and angles ( ) for $NH_4B_{11}O_{16}(OH)_2$.

B(1)−O(5)	1.351(4)	B(4)−O(6)	1.373(4)
B(1)−O(2)	1.372(4)	B(4)−O(5)	1.374(3)
B(1)−O(4)	1.374(4)	B(5)−O(9)	1.328(4)
B(2)−O(8)	1.349(4)	B(5)−O(8)	1.370(4)
B(2)−O(3)	1.361(4)	B(5)−O(6)#1	1.384(3)
B(2)−O(4)	1.369(4)	B(6)−O(7)#2	1.460(3)
B(3)−O(1)	1.344(4)	B(6)−O(7)	1.460(3)
B(3)−O(3)	1.372(4)	B(6)−O(9)#3	1.471(3)
B(3)−O(2)	1.384(3)	B(6)−O(9)#4	1.471(3)
B(4)−O(7)	1.329(4)		
O(5)−B(1)−O(2)	123.9(3)	O(6)−B(4)−O(5)	119.6(3)
O(5)−B(1)−O(4)	116.0(3)	O(9)−B(5)−O(8)	126.1(3)
O(2)−B(1)−O(4)	120.1(2)	O(9)−B(5)−O(6)#1	121.9(3)
O(8)−B(2)−O(3)	118.0(3)	O(8)−B(5)−O(6)#1	112.0(3)
O(8)−B(2)−O(4)	121.8(3)	O(7)#2−B(6)−O(7)	107.2(3)
O(3)−B(2)−O(4)	120.1(3)	O(7)#2−B(6)−O(9)#3	111.72(10)
O(1)−B(3)−O(3)	122.3(3)	O(7)−B(6)−O(9)#3	109.11(10)
O(1)−B(3)−O(2)	117.9(3)	O(7)#2−B(6)−O(9)#4	109.11(10)
O(3)−B(3)−O(2)	119.8(3)	O(7)−B(6)−O(9)#4	111.72(10)
O(7)−B(4)−O(6)	122.0(3)	O(9)#3−B(6)−O(9)#4	108.0(3)
O(7)−B(4)−O(5)	118.4(3)		

Symmetry transformations used to generate equivalent atoms:

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

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

Table S3. Hydrogen bond lengths (Å) and angles (°) for $NH_4B_{11}O_{16}(OH)_2$**.** D, hydrogen bond donor; A, hydrogen bond acceptor.

D−H ··A	$d_{(D-H)}$	$d_{(H\cdots A)}$	$d_{(D\cdots A)}$	$<_{(D-H\cdots A)}$
O1−H1 ··O9	0.820	2.258	3.010	152.63
N1−H2 ··O8	0.956	2.040	2.973	164.72
N1−H3 ··O6	0.854	2.339	2.825	116.45
N1−H3 ··O7	0.854	2.566	2.995	112.16

Table S4. Configurations of the fundamental building blocks (FBBs) for known ammonium borates and their number ratios of hydroxyl groups to boron atoms.

Ammonium Borates	FBB Configurations	N_{OH}/N_B
$(NH_4)_2[B_4O_5(OH)_4]\cdot 2H_2O$	$\{4:[<2\Delta 2T>^{b}]\}$	1
$NH_4[B_5O_6(OH)_4]\cdot 2H_2O$	$\{5:[<4\Delta T>^{8}]\}$	0.8
$(NH_4)_3[B_{15}O_{20}(OH)_8]\cdot 4H_2O$	$\{15:[3<4\Delta T>^{8}]\}$	0.53
$NH_4[B_5O_7(OH)_2]\cdot H_2O$	$\{5:_{\infty}^{1}[<4\Delta T>^{8}]\}$	0.4
$(NH_4)_2[B_{10}O_{14}(OH)_4]\cdot H_2O$	$\{10:_{\infty}^{1}[2<4\Delta T>^{8}]\}$	0.4
$NH_4B_{11}O_{16}(OH)_2$	$\{11:_{\infty}^{2}[<3\Delta>+<4\Delta T>^{8}+<3\Delta>]\}$	0.18
HP-$NH_4B_3O_5$	$\{3:_{\infty}^{3}[<\Delta 2T>]\}$	0
$NH_4B_5O_8$	$\{5:_{\infty}^{3}[<4\Delta T>^{8}]\}$	0

Note: the superscript “b” expresses the bridge-ring FBB, and the superscript “8” expresses the ‘8’-shaped-ring FBB.

Figure S1. Two kinds of hydrogen bonds and their connection environments. Notations of D and A means hydrogen bond donors and acceptors, respectively, for O atoms which are involved in hydrogen bonds (O−H···O and N−H···O).