Supporting Information

New Fluoroborate $Cd_8B_5O_{15}F$ with Two Different Isolated Borate Anions Prepared by an Open High-Temperature Solution Method

Yun Yang,[a] Xiaoyu Dong[a,b] and Shilie Pan[a]*

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

[b] Engineering Department of Chemistry and Environment, Xinjiang Institute of Engineering, 236 Nanchang Road, Urumqi 830091, China

Figure S1. TG/DSC curves of $Cd_8B_5O_{15}F$.

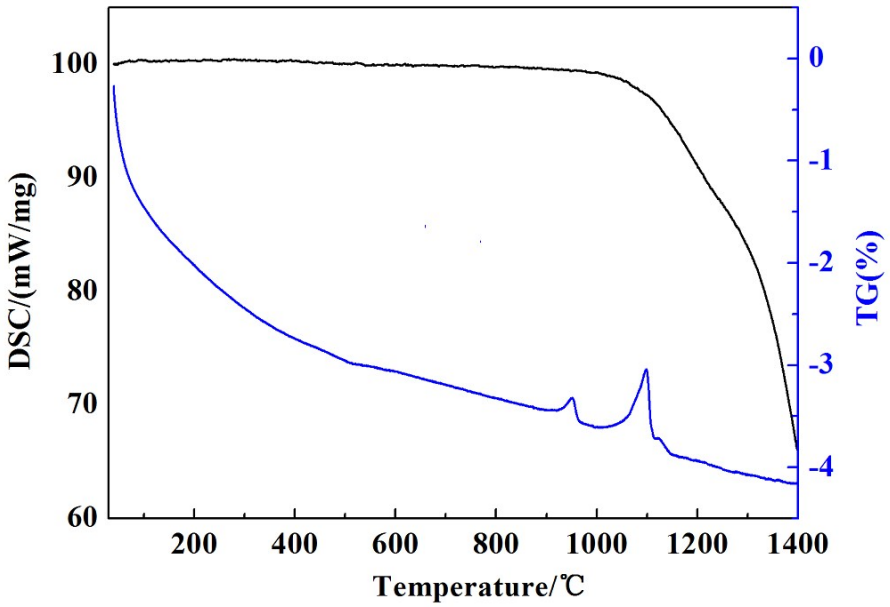

Figure S2. Infrared spectroscopy of the $Cd_8B_5O_{15}F$ sample.

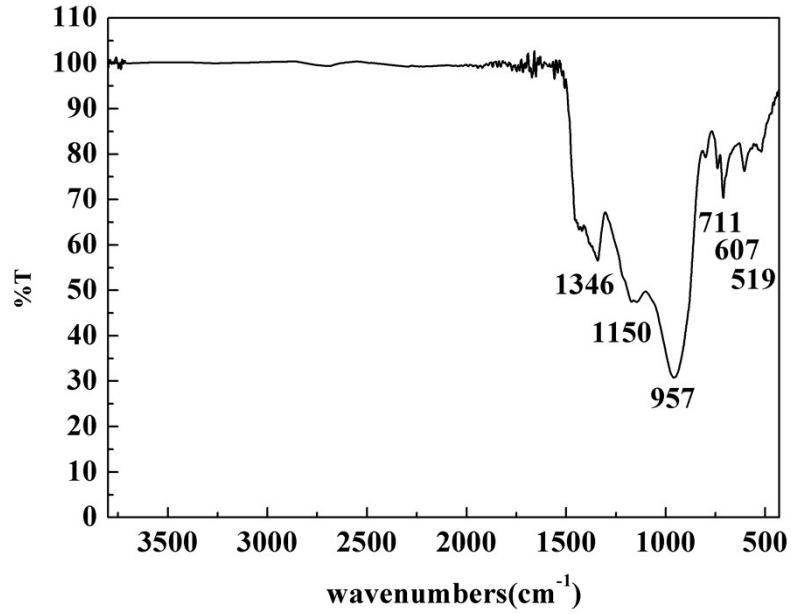

Figure S3. XPS spectra of F1s of the $Cd_8B_5O_{15}F$ sample.

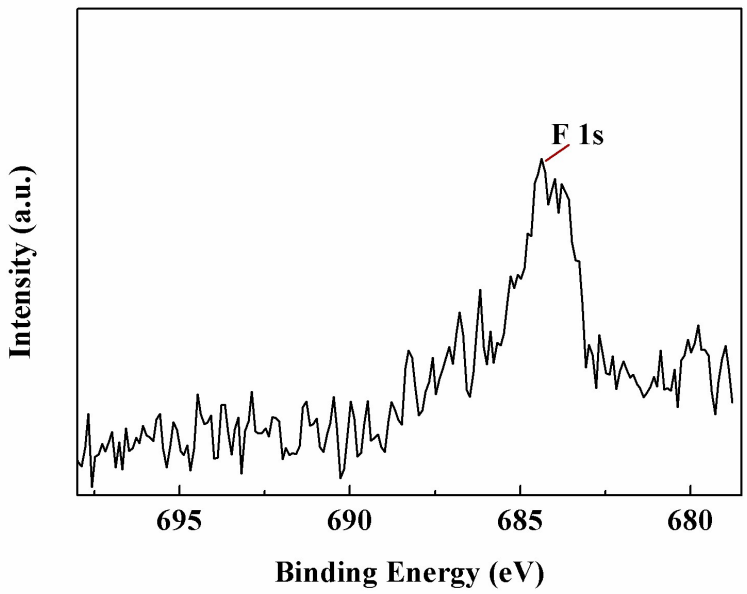

Figure S4. FT-Raman spectrum of $Cd_8B_5O_{15}F$.

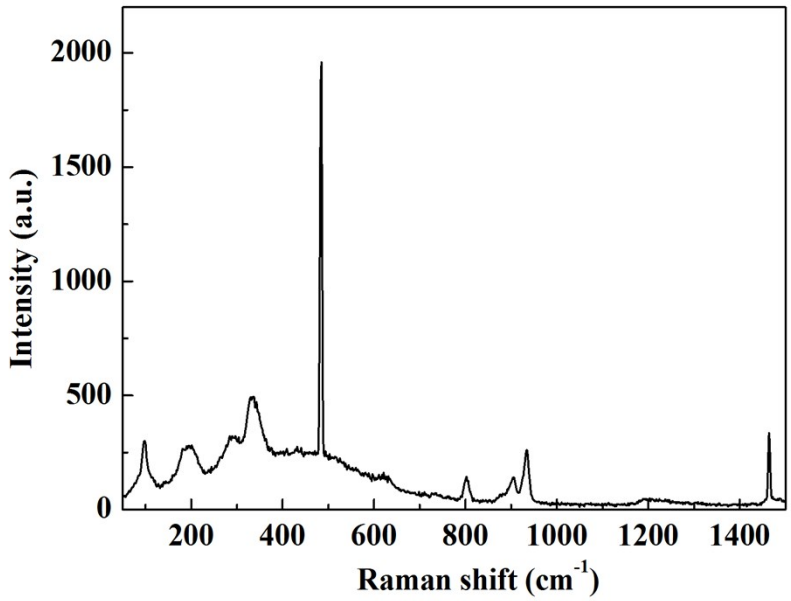

Table S1. Selected bond distances (Å) and angles (deg) for $Cd_8B_5O_{15}F$.

Cd(1))-O(2)#1	2.281(12)	Cd(2))-O(2)#8	2.320 (13)
Cd(1))-O(2)#2	2.281(12)	Cd(2))-O(2)#9	2.320(13)
Cd(1))-O(2)#3	2.281(12)	Cd(2))-O(2)#10	2.320(13)
Cd(1))-O(2)#4	2.281(12)	Cd(2))-O(2)#2	2.320(13)
Cd(1))-O(2)#5	2.307(14)	Cd(2))-O(2)#11	2.320(13)
Cd(1))-O(2)	2.307(14)	Cd(2))-O(2)#12	2.320(13)
Cd(1))-O(2)#6	2.307(14)	Cd(2))-O(2)#4	2.320(13)
Cd(1))-O(2)#7	2.307(14)	Cd(2))-O(2)#7	2.320(13)
Cd(1))-F(1))#6	2.394(3)	Cd(2))-O(2)#13	2.320(13)
Cd(1))-O(1)#6	2.394(3)	Cd(2))-O(2)	2.320(13)
Cd(1))-O(1)	2.394(3)	Cd(2))-O(2)#14	2.320(13)
B(1))-O(1)	1.47(2)	Cd(2))-O(2)#15	2.320(13)
B(1))-F(1))	1.47(2)	B(2))-O(2)	1.352(14)
B(1))-O(1)#19	1.47(2)	B(2))-O(2)#5	1.352(14)
B(1))-F(1))#19	1.47(2)	B(2))-O(2)#21	1.352(14)
B(1))-O(1)#20	1.47(2)	B(1))-O(1)#6	1.47(2)
B(1))-F(1))#20	1.47(2)	B(1))-F(1))#6	1.47(2)
O(2)#1-Cd(1))-O(2)#2	174.9(7)	O(2)#2-Cd(1))-O(2)#4	31.6(7)
O(2)#1-Cd(1))-O(2)#3	31.6(7)	O(2)#3-Cd(1))-O(2)#4	174.9(7)
O(2)#2-Cd(1))-O(2)#3	148.0(7)	O(2)#1-Cd(1))-O(2)#5	59.9(6)
O(2)#1-Cd(1))-O(2)#4	148.0(7)	O(2)#2-Cd(1))-O(2)#5	115.9(3)
O(2)#3-Cd(1))-O(2)#5	80.1(6)	O(2)#4-Cd(1))-O(2)#5	96.1(3)
O(2)#1-Cd(1))-O(2)	96.1(3)	O(2)#2-Cd(1))-O(2)	80.1(6)
O(2)#3-Cd(1))-O(2)	115.9(3)	O(2)#4-Cd(1))-O(2)	59.9(6)
O(2)#5-Cd(1))-O(2)	36.9(7)	O(2)#1-Cd(1))-O(2)#6	80.1(6)
O(2)#2-Cd(1))-O(2)#6	96.1(3)	O(2)-Cd(1))-O(2)#6	86.2(6)
O(2)#3-Cd(1))-O(2)#6	59.9(6)	O(2)#1-Cd(1))-O(2)#7	115.9(3)
O(2)#4-Cd(1))-O(2)#6	115.9(3)	O(2)#2-Cd(1))-O(2)#7	59.9(6)
O(2)#5-Cd(1))-O(2)#6	74.5(6)	O(2)#3-Cd(1))-O(2)#7	96.1(3)
O(2)#4-Cd(1))-O(2)#7	80.1(6)	O(2)#5-Cd(1))-O(2)#7	86.2(6)
O(2)-Cd(1))-O(2)#7	74.5(6)	O(2)#6-Cd(1))-O(2)#7	36.9(7)
O(2)#1-Cd(1))-F(1))#6	100.1(4)	O(2)#2-Cd(1))-F(1))#6	84.4(4)
O(2)#3-Cd(1))-F(1))#6	84.4(4)	O(2)#4-Cd(1))-F(1))#6	100.1(4)
O(2)#5-Cd(1))-F(1))#6	159.3(4)	O(2)-Cd(1))-F(1))#6	159.3(4)
O(2)#6-Cd(1))-F(1))#6	109.3(6)	O(2)#7-Cd(1))-F(1))#6	109.3(6)
O(2)#1-Cd(1))-O(1)#6	100.1(4)	O(2)#2-Cd(1))-O(1)#6	84.4(4)
O(2)#3-Cd(1))-O(1)#6	84.4(4)	O(2)#4-Cd(1))-O(1)#6	100.1(4)
O(2)#5-Cd(1))-O(1)#6	159.3(4)	O(2)-Cd(1))-O(1)#6	159.3(4)
O(2)#6-Cd(1))-O(1)#6	109.3(6)	O(2)#7-Cd(1))-O(1)#6	109.3(6)
F(1))#6-Cd(1))-O(1)#6	0.0(3)	O(2)#1-Cd(1))-O(1)	84.4(4)
O(2)#2-Cd(1))-O(1)	100.1(4)	O(2)#3-Cd(1))-O(1)	100.1(4)
O(2)#4-Cd(1))-O(1)	84.4(4)	O(2)#5-Cd(1))-O(1)	109.3(6)
O(2)-Cd(1))-O(1)	109.3(6)	O(2)#6-Cd(1))-O(1)	159.3(4)
O(2)#7-Cd(1))-O(1)	159.3(4)	F(1))#6-Cd(1))-O(1)	60.0(11)
O(1)#6-Cd(1))-O(1)	60.0(11)	O(2)#8-Cd(2))-O(2)#9	31.0(7)
O(2)#8-Cd(2))-O(2)#10	59.2(7)	O(2)#9-Cd(2))-O(2)#10	79.0(4)

O(2)#8-Cd(2))-O(2)#2	101.0(4)	O(2)#9-Cd(2))-O(2)#2	120.8(7)
O(2)#10-Cd(2))-O(2)#2	106.0(6)	O(2)#8-Cd(2))-O(2)#11	120.8(7)
O(2)#9-Cd(2))-O(2)#11	101.0(4)	O(2)#10-Cd(2))-O(2)#11	180.000(1)
O(2)#2-Cd(2))-O(2)#11	74.0(6)	O(2)#8-Cd(2))-O(2)#12	79.0(4)
O(2)#9-Cd(2))-O(2)#12	59.2(7)	O(2)#10-Cd(2))-O(2)#12	74.0(6)
O(2)#2-Cd(2))-O(2)#12	180.000(1)	O(2)#11-Cd(2))-O(2)#12	106.0(6)
O(2)#8-Cd(2))-O(2)#4	74.0(6)	O(2)#9-Cd(2))-O(2)#4	101.0(4)
O(2)#10-Cd(2))-O(2)#4	79.0(4)	O(2)#2-Cd(2))-O(2)#4	31.0(7)
O(2)#11-Cd(2))-O(2)#4	101.0(4)	O(2)#12-Cd(2))-O(2)#4	149.0(7)
O(2)#8-Cd(2))-O(2)#7	149.0(7)	O(2)#9-Cd(2))-O(2)#7	180.00(19)
O(2)#10-Cd(2))-O(2)#7	101.0(4)	O(2)#2-Cd(2))-O(2)#7	59.2(7)
O(2)#11-Cd(2))-O(2)#7	79.0(4)	O(2)#12-Cd(2))-O(2)#7	120.8(7)
O(2)#4-Cd(2))-O(2)#7	79.0(4)	O(2)#8-Cd(2))-O(2)#13	180.000(1)
O(2)#9-Cd(2))-O(2)#13	149.0(7)	O(2)#10-Cd(2))-O(2)#13	120.8(7)
O(2)#2-Cd(2))-O(2)#13	79.0(4)	O(2)#11-Cd(2))-O(2)#13	59.2(7)
O(2)#12-Cd(2))-O(2)#13	101.0(4)	O(2)#4-Cd(2))-O(2)#13	106.0(7)
O(2)#7-Cd(2))-O(2)#13	31.0(7)	O(2)#8-Cd(2))-O(2)	79.0(4)
O(2)#9-Cd(2))-O(2)	106.0(6)	O(2)#10-Cd(2))-O(2)	31.0(7)
O(2)#2-Cd(2))-O(2)	79.0(4)	O(2)#11-Cd(2))-O(2)	149.0(7)
O(2)#12-Cd(2))-O(2)	101.0(4)	O(2)#4-Cd(2))-O(2)	59.2(7)
O(2)#7-Cd(2))-O(2)	74.0(6)	O(2)#13-Cd(2))-O(2)	101.0(4)
O(2)#8-Cd(2))-O(2)#14	101.0(4)	O(2)#9-Cd(2))-O(2)#14	74.0(6)
O(2)#10-Cd(2))-O(2)#14	149.0(7)	O(2)#2-Cd(2))-O(2)#14	101.0(4)
O(2)#11-Cd(2))-O(2)#14	31.0(7)	O(2)#12-Cd(2))-O(2)#14	79.0(4)
O(2)#4-Cd(2))-O(2)#14	120.8(7)	O(2)#7-Cd(2))-O(2)#14	106.0(6)
O(2)#13-Cd(2))-O(2)#14	79.0(4)	O(2)-Cd(2))-O(2)#14	180.0(6)
O(2)#8-Cd(2))-O(2)#15	106.0(7)	O(2)#9-Cd(2))-O(2)#15	79.0(4)
O(2)#10-Cd(2))-O(2)#15	101.0(4)	O(2)#2-Cd(2))-O(2)#15	149.0(7)
O(2)#11-Cd(2))-O(2)#15	79.0(4)	O(2)#12-Cd(2))-O(2)#15	31.0(7)
O(2)#4-Cd(2))-O(2)#15	180.0(6)	O(2)#7-Cd(2))-O(2)#15	101.0(4)
O(2)#13-Cd(2))-O(2)#15	74.0(6)	O(2)-Cd(2))-O(2)#15	120.8(7)
O(2)#14-Cd(2))-O(2)#15	59.2(7)	O(1)-B(1))-F(1))#19	109.471(2)
O(1)-B(1))-O(1)#19	109.471(2)	F(1))#19-B(1))-O(1)#19	0.0(18)
O(1)-B(1))-F(1))#20	109.5	F(1))#19-B(1))-F(1))#20	109.5
O(1)#19-B(1))-F(1))#20	109.5	O(1)-B(1))-O(1)#20	109.5
F(1))#19-B(1))-O(1)#20	109.5	O(1)#19-B(1))-O(1)#20	109.5
F(1))#20-B(1))-O(1)#20	0.0(18)	O(1)-B(1))-O(1)#6	109.471(1)
F(1))#19-B(1))-O(1)#6	109.471(6)	O(1)#19-B(1))-O(1)#6	109.471(6)
F(1))#20-B(1))-O(1)#6	109.471(2)	O(1)#20-B(1))-O(1)#6	109.471(2)
O(1)-B(1))-F(1))#6	109.471(1)	F(1))#19-B(1))-F(1))#6	109.471(6)
O(1)#19-B(1))-F(1))#6	109.471(6)	F(1))#20-B(1))-F(1))#6	109.471(2)
O(1)#20-B(1))-F(1))#6	109.471(2)	O(1)#6-B(1))-F(1))#6	0.0(18)
O(2)#5-B(2))-O(2)#21	119.95(11)	O(2)#5-B(2))-O(2)	65.3(12)
O(2)#21-B(2))-O(2)	174.1(16)	O(2)#5-B(2))-O(2)#22	174.1(16)

O(2)#21-B(2))-O(2)#22	54.7(12)	O(2)-B(2))-O(2)#22	119.95(11)
O(2)#5-B(2))-O(2)#23	54.7(12)	O(2)#21-B(2))-O(2)#23	65.3(12)
O(2)-B(2))-O(2)#23	119.95(11)	O(2)#22-B(2))-O(2)#23	119.95(11)
O(2)#5-B(2))-O(2)#10	119.95(11)	O(2)#21-B(2))-O(2)#10	119.95(11)
O(2)-B(2))-O(2)#10	54.7(12)	O(2)#22-B(2))-O(2)#10	65.3(12)
O(2)#23-B(2))-O(2)#10	174.1(16)		

#1 -y+1/2,-z+1/2,-x
#2 y-1/4,-z+1/2,x+1/4
#3 x+1/4,-z+1/2,y-1/4
#4 -x,-z+1/2,-y+1/2
#5 z,y,x
#6 -x+1/4,y,-z+1/4
#7 -z+1/4,y,-x+1/4
#8 z-1/4,x+1/4,-y+1/2
#9 z-1/4,-y+1/2,x+1/4
#10 -y+1/4,-x+1/4,z
#11 y-1/4,x+1/4,-z+1/2
#12 -y+1/4,z,-x+1/4
#13 -z+1/4,-x+1/4,y
#14 -x,-y+1/2,-z+1/2
#15 x,z,y
#16 z,x+1/2,y-1/2
#17 y-1/2,z+1/2,x
#18 -z,-x+1/2,-y+1/2
#19 -x+1/4,-y+5/4,z
#20 x,-y+5/4,-z+1/4
#21 x,-z+1/4,-y+1/4
#22 -y+1/4,-z+1/4,x
#23 z,-x+1/4,-y+1/4

Table S2. Bond valence analysis of $Cd_8B_5O_{15}F$.[a,b]

Atoms	l	s	Atoms	l	s
Cd(1)-O(1)	2.394	0.1995	B(1)-O(1)	1.467	0.57825
Cd(1)-O(1)	2.394	0.1995	B(1)-O(1)	1.467	0.57825
Cd(1)-O(2)	2.281	0.361	B(1)-O(1)	1.467	0.57825
Cd(1)-O(2)	2.281	0.361	B(1)-O(1)	1.467	0.57825
Cd(1)-O(2)	2.307	0.336	B(1)-F(1)	1.467	0.15125
Cd(1)-O(2)	2.307	0.336	B(1)-F(1)	1.467	0.15125
Cd(1)-F(1)	2.394	0.04375	B(1)-F(1)	1.467	0.15125
Cd(1)-F(1)	2.394	0.04375	B(1)-F(1)	1.467	0.15125
∑s		1.8805	∑s		2.918
Cd(2)-O(2)	2.321	0.324	B(2)-O(2)	1.352	1.053
Cd(2)-O(2)	2.321	0.324	B(2)-O(2)	1.352	1.053
Cd(2)-O(2)	2.321	0.324	B(2)-O(2)	1.352	1.053
Cd(2)-O(2)	2.321	0.324	∑s		3.159
Cd(2)-O(2)	2.321	0.324	F(1)-Cd(1)	2.394	0.175
Cd(2)-O(2)	2.321	0.324	F(1)-Cd(1)	2.394	0.175
∑s		1.944	F(1)-Cd(1)	2.394	0.175
			F(1)-B1	1.467	0.605
			∑s		1.13

[a] Bond valences calculated with the program Bond Valence Calculator Version 2.00, Hormillosa, C., Healy, S., Stephen, T. McMaster University (1993).

[b] Valence sums calculated with the formula: Si = exp[(R0-Ri)/B], where Si = valence of bond "i" and B = 0.37. Superscripts indicate the number of equivalent bonds for anions.