Supporting Information

Discovery of a New Bimetallic Borate with Strong Optical Anisotropy Activated by

π-conjugated [B₂O₅] units

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Experimental Section

Regents. SrF_2 (99%), CdF_2 (99%), and H_3BO_3 (99%) were acquired commercially and used directly as raw materials without further purification.

Single crystal preparation and the synthesis of compounds. single crystal $Sr_2Cd_4(B_2O_5)_3$ was grown by the high-temperature solution method in the open environment. Weighed on an analytical balance in the stoichiometric ratio SrF_2 : CdF_2 : H_3BO_3 = 1 : 2 : 4, the mixtures were ground thoroughly, loaded into a platinum crucible, which was placed in a vertical programmable temperature furnace. Gradually hated from normal atmospheric temperature to 850 °C in 500 min, the samples were calcined at a preset for 72 h and then slowly cooled to normal atmospheric temperature at 6 °C/h. Colorless crystals of $Sr_2Cd_4(B_2O_5)_3$ were obtained, single crystals with a high quality and proper sizes were selected from the batch to further determine their respective average structures. Power sample of $Sr_2Cd_4(B_2O_5)_3$ was synthesized by solid-state reaction method in the open environment. Weighed on an analytical balance in the stoichiometric ratio of $SrCO_3$: $CdCO_3$: B_2O_3 = 1 : 2 : 1.5, and these mixtures were thoroughly ground in an agate mortar, then transferred to a corundum crucible and placed in a pure sample furnace. These mixtures are heated to 500 °C, pre-fired at 500 °C for a period of time, then gradually heated to 800 °C and held for 72 h. Repeating the grinding and mixing several times during this period, a pure sample of $Sr_2Cd_4(B_2O_5)_3$ polycrystalline powder was finally obtained.

Characterization. Powder XRD data were collected with a Bruker D2 PHASER diffractometer (Cu Kα radiation with λ = 1.5418 Å, 2θ = 10 to 70°, scan step width = 0.02°, and counting time= 1 s/step). The single-crystal XRD data were collected on a Bruker D8 Venture diffractometer using Mo Kα radiation (λ = 0.71073 Å) at room temperature. The intensity, reduction and cell refinement were carried out on Bruker SAINT.[1] All the structures were solved by direct method and refined through the full matrix least-squares fitting on F^2 with OLEX2 software.[2] These structures were verified by virtue of ADDSYM algorithm from PLATON.[3] UV−Vis−NIR diffuse-reflectance spectroscopy data in the wavelength range of 250-2500 nm were recorded at room temperature using a powder sample of $Sr_2Cd_4(B_2O_5)_3$ on a Shimadzu SolidSpec-3700 DUV spectrophotometer. Thermal properties characterized by using a NETZSCH STA 449F3 simultaneous analyzer with a heating rate of 5 °C/min a nitrogen atmosphere.

Calculation details. The electronic structure and optical property were calculated by using the DFT method implemented in the CASTEP package.[4] During the calculation, the

generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional was adopted.[5] Under the norm-conserving pseudopotential (NCP), the following orbital electrons were treated as valence electrons: $B:2s^22p^1$, $O:2s^22p^4$, $Sr:4s^24p^65s^1$, $Cd: 4d^{10}5s^2$. The kinetic energy cutoffs of 800 eV were chosen, and the numerical integration of the Brillouin zone was performed using a $3 \times 3 \times 4$ Monkhorst-Pack k-point sampling. A $1\times 1\times 2$ supercell is created on the basis of a single cell of $Sr_2Cd_4(B_2O_5)_3$ and the relevant calculations are performed. The other calculation parameters and convergent criteria were the default values of the CASTEP code. Although the GGA-PBE method is adequately eligible to describe the electronic structures and optical properties in terms of numerous crystals. The scissors operation was used here to simulate the electric field of the real condition strictly.

The birefringence is proportional to the REDA index,[6] and the formula can be expressed as:

$$\Delta n = \frac{R\Sigma_g[NcZa\Delta\rho^b]_g}{2n_1E_o}$$

Where, R is the correction coefficient, N_c is the coordination number of the nearest neighbor cations to the central anion, Z_a is the formal chemical valence of the anion and E_o is the optical bandgap; $\Delta\rho^b = \rho max^b - \rho min^b$, ρmax^b and ρmin^b are the maximum and minimum of the covalent electron density of the covalent bond on the optical principal axes of a crystal, and n_1 is the minimum refractive index.

The coordination of metal cations and six oxygen atoms often forms the octahedra of MO_6, but these octahedra are often structurally distorted due to the SOJT effect, and in this paper the calculation of the octahedral distortion proposed by Halasyamani[7]:

$$\Delta d = \frac{|(M-O1)-(M-O4)|}{|\cos\theta_1|} + \frac{|(M-O2)-(M-O5)|}{|\cos\theta_2|} + \frac{|(M-O3)-(M-O6)|}{|\cos\theta_3|}$$

no distortion: Δd = 0.00-0.05, weak distortion: Δd = 0.05-0.40, moderate distortion: Δd = 0.40-0.80, strong distortion: $\Delta d > 0.80$.

Table S1. The basic information of the existing zinc borates

Dimension	Chemical formula	Space group	B-O cluster
0D	$Pb_2Ba_4Zn_4(B_2O_5)(B_6O_{13})_2$	$P1$	$[B_2O_5] + [B_6O_{13}]$
0D	$Ba_2ZnSc(BO_3)_3$	$P\bar{1}$	$[BO_3]$
0D	$Ba_2Zn(B_3O_6)_2$	$P\bar{1}$	$[B_3O_6]$
0D	$LiZn(BO_3)$	$P\bar{1}$	$[BO_3]$
0D	$Zn_3(BO_3)_2$	$P\bar{1}$	$[BO_3]$
0D	$K_2Zn_2(B_6O_{12})$	$P\bar{1}$	$[B_6O_{12}]$
0D	$Ba_5Zn_4(BO_3)_6$	Pc	$[BO_3]$
0D	$Pb_2Ba_4Zn_4(B_2O_5)(B_6O_{13})_2$	Cc	$[B_2O_5] + [B_6O_{13}]$
0D	$BaLiZn_3(BO_3)_3$	$P2/c$	$[BO_3]$
0D	$CsZn_4(BO_3)_3$	$P2/c$	$[BO_3]$
0D	$KZn_4(BO_3)_3$	$P2/c$	$[BO_3]$
0D	$RbZn_4(BO_3)_3$	$P2/c$	$[BO_3]$
0D	$Ba_4Zn_5Sc_2(BO_3)_8$	$P2_1/c$	$[BO_3]$
0D	$K_3Zn(B_5O_{10})$	$P2_1/c$	$[B_5O_{10}]$
0D	$Na_3Zn(B_5O_{10})$	$P2_1/c$	$[B_5O_{10}]$
0D	$Rb_3Zn(B_5O_{10})$	$P2_1/c$	$[B_5O_{10}]$
0D	$Ba_3Zn_2(BO_3)_3F$	$P2_1/c$	$[BO_3]$
0D	$K_2NaZn(B_5O_{10})$	$C2/c$	$[B_5O_{10}]$
0D	$Zn_3(BO_3)_2$	$C2/c$	$[BO_3]$
0D	$LiZn(BO_3)$	$C2/c$	$[BO_3]$
0D	$Ba_3Zn_2(BO_3)_4F_2$	$C2/c$	$[BO_3]$
0D	$BaZn_2(BO_3)_2$	$P2_12_12_1$	$[BO_3]$
0D	$Ba_2Zn(BO_3)_2$	$Pca2_1$	$[BO_3]$
0D	$Bi_2Zn(B_2O_5)O_2$	$Pba2$	$[B_2O_5]$
0D	$Cs_3Zn_6(B_3O_6)_2(BO_3)_3$	$Cmc2_1$	$[BO_3] + [B_3O_6]$
0D	$CaZn_2(BO_3)_2$	$Aba2$	$[BO_3]$
0D	$PbZn_2(BO_3)_2$	$Pccn$	$[BO_3]$
0D	$Na_3Zn(B_5O_{10})$	$Pbca$	$[B_5O_{10}]$
0D	$Ba_3Zn_2(BO_3)_3F$	$Pnma$	$[BO_3]$
0D	$Pb_2Ba_4Zn_4(B_2O_5)(B_6O_{13})_2$	$P3_2$	$[B_2O_5] + [B_6O_{13}]$
0D	$CsZn_2BO_3FCl$	$R3$	$[BO_3]$
0D	$BaZnBe_2(BO_3)_2F_2$	$P\bar{3}$	$[BO_3]$

Table S1. The basic information of the existing zinc borates (continued)

Dimension	Chemical formula	Space group	B-O cluster
0D	$BaZn_3(BO_3)_2F_2$	$P3$	$[BO_3]$
0D	$KZn_2(BO_3)Cl_2$	$R32$	$[BO_3]$
0D	$KZn_2(BO_3)Br_2$	$R32$	$[BO_3]$
0D	$RbZn_2(BO_3)Br_2$	$R32$	$[BO_3]$
0D	$RbZn_2(BO_3)Cl_2$	$R32$	$[BO_3]$
0D	$K_7ZnSc_2(B_5O_{10})_3$	$R32$	$[B_5O_{10}]$
0D	$CsZn_2BO_3F_2$	$R32$	$[BO_3]$
0D	$CsZn_2BO_3Cl_2$	$R32$	$[BO_3]$
0D	$CdZn_2(BO_3)_2$	$R3c$	$[BO_3]$
0D	$Cd_3Zn_3(BO_3)_4$	$R3c$	$[BO_3]$
0D	$CdZn_2K(BO_3)_2F$	$P\bar{3}1c$	$[BO_3]$
0D	$BaZn(BO_3)F$	$P\bar{6}$	$[BO_3]$
2D	$Na_2ZnB_6O_{11}$	Cc	$[BO_3] + [BO_4]$
2D	$EuZnB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$LaZnB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$CeZnB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$NdZnB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$TbZnB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$GdZnB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$YZnB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$Pb_4Zn_2B_{10}O_{21}$	$Pbcn$	$[BO_3] + [BO_4]$
3D	$Zn_3B_7O_{13}Br$	$Pca2_1$	$[BO_3] + [BO_4]$
3D	ZnB_4O_7	$Pbca$	$[BO_3] + [BO_4]$
3D	ZnB_4O_7	$Cmcm$	$[BO_4]$
3D	$Zn_3B_7O_{13}Cl$	$R3c$	$[BO_3] + [BO_4]$
3D	$Zn_8Se_2B_{12}O_{24}$	$I\bar{4}3m$	$[BO_4]$
3D	$Zn_4B_6O_{13}$	$I\bar{4}3m$	$[BO_4]$

Table S2. The basic information of the existing cadmium borates

Dimension	Chemical formula	Space group	B-O cluster
0D	$Cd_3(BO_3)_2$	$P\bar{1}$	$[BO_3]$
0D	$LiCd(BO_3)$	$P\bar{1}$	$[BO_3]$
0D	$Cd_2(B_2O_5)$	$P\bar{1}$	$[B_2O_5]$
0D	$Ba_2CdSc(BO_3)_3$	$P\bar{1}$	$[BO_3]$
0D	$Cd_4BiO(BO_3)_3$	Cm	$[BO_3]$
0D	$Cd_5(BO_3)_3Cl$	Cm	$[BO_3]$
0D	$Cd_4DyO(BO_3)_3$	Cm	$[BO_3]$
0D	$Cd_4GdO(BO_3)_3$	Cm	$[BO_3]$
0D	$Cd_4EuO(BO_3)_3$	Cm	$[BO_3]$
0D	$Ba_2Cd(BO_3)_2$	$C2/m$	$[BO_3]$
0D	$LiCd(BO_3)$	$P2_1/c$	$[BO_3]$
0D	$K_3Cd(B_5O_{10})$	$P2_1/c$	$[B_5O_{10}]$
0D	$Rb_3Cd(B_5O_{10})$	$P2_1/c$	$[B_5O_{10}]$
0D	$Ba_2CdY_2(BO_3)_4$	$P2_1/c$	$[BO_3]$
0D	$Cu_2Cd(B_2O_5)O$	$P2_1/c$	$[B_2O_5]$
0D	$KCd(B_3O_6)$	$C2/c$	$[B_3O_6]$
0D	$RbCd(B_3O_6)$	$C2/c$	$[B_3O_6]$
0D	$SrCd(B_2O_5)$	$C2/c$	$[B_2O_5]$
0D	$Cd_3(BO_3)_2$	$Pnnm$	$[BO_3]$
0D	$SrCd(B_2O_5)$	$Pbca$	$[B_2O_5]$
0D	$Cd_{12}Ge_{17}(B_2O_7)_4O_{44}$	P	$[B_2O_7]$
0D	$Cu_2Cd(B_2O_5)O$	$P2_1/c$	$[B_2O_5]$
0D	$KCd(B_3O_6)$	$C2/c$	$[B_3O_6]$
0D	$RbCd(B_3O_6)$	$C2/c$	$[B_3O_6]$
0D	$SrCd(B_2O_5)$	$C2/c$	$[B_2O_5]$
0D	$Cd_3(BO_3)_2$	$Pnnm$	$[BO_3]$
0D	$SrCd(B_2O_5)$	$Pbca$	$[B_2O_5]$
0D	$Cd_{12}Ge_{17}(B_2O_7)_4O_{44}$	$P\bar{4}$	$[B_2O_7]$
0D	$Cd_6Na_8Li_2Be_8(B_{12}O_2BO_3)_8F_2$	$R\bar{3}$	$[BO_3] + [B_{12}O_{24}]$
0D	$Ba_2Cd(B_3O_6)_2$	$R\bar{3}$	$[B_3O_6]$

Table S2. The basic information of the existing cadmium borates (continued)

Dimension	Chemical formula	Space group	B-O cluster
0D	$K_7CdGd_2(B_5O_{10})_3$	$R32$	$[B_5O_{10}]$
0D	$K_7CdLu_2(B_5O_{10})_3$	$R32$	$[B_5O_{10}]$
0D	$K_7CdSc_2(B_5O_{10})_3$	$R32$	$[B_5O_{10}]$
0D	$K_7CdY_2(B_5O_{10})_3$	$R32$	$[B_5O_{10}]$
0D	$CdZn_2(BO_3)_2$	$R3c$	$[BO_3]$
0D	$Cd_3Zn_3(BO_3)_4$	$R3c$	$[BO_3]$
0D	$CdZn_2K(BO_3)_2F$	$P\bar{3}1c$	$[BO_3]$
0D	$LiCd(BO_3)$	$p\bar{6}$	$[BO_3]$
0D	$EuCd_3(AlO)_3(BO_3)_4$	$P6_3$	$[BO_3]$
0D	$Pb_3Cd_3(BO_3)_4$	$P6_3/m$	$[BO_3]$
0D	$LiCdY_5(BO_3)_6$	$P6_522$	$[BO_3]$
0D	$CsCd(BO_3)$	$P2_13$	$[BO_3]$
2D	$PbCd_2B_6O_{12}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$CdEuB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$CdLaB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$CdSmB_5O_{10}$	$P2_1/c$	$[BO_3] + [BO_4]$
2D	$Cd_3Cs_2B_{16}O_{28}$	$C2/c$	$[BO_3] + [BO_4]$
2D	$Cd_3Rb_2B_{16}O_{28}$	$C2/c$	$[BO_3] + [BO_4]$
3D	CdB_4O_7	$Pbca$	$[BO_3] + [BO_4]$
3D	CdB_2O_4	$P6_3$	$[BO_3] + [BO_4]$

Table S3. Crystallographic data and structure refinement parameters of $Sr_2Cd_4(B_2O_5)_3$.

Compound	$Sr_2Cd_4(B_2O_5)_3$
Formula weight	929.70
Temperature/K	299.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.6878(11)
b/Å	5.2551(4)
c/Å	11.5527(12)
α/°	90
β/°	92.154(4)
γ/°	90
Volume/Å^3	648.40(11)
Z	2
ρ_{calc} g/cm^3	4.762
μ/mm^{-1}	14.697
F(000)	836.0
Radiation	MoKα ($\lambda = 0.71073$)
2θ range for data collection/°	3.814 to 55.022
Completeness (%)	99.9
Index ranges	$-13 \leq h \leq 13, -6 \leq k \leq 6, -14 \leq l \leq 15$
Reflections collected	4541
Independent reflections	1455 [$R_{int}= 0.0690$, $R_{sigma}= 0.0648$]
Data/restraints/parameters	1455/0/128
Goodness-of-fit on F^2	1.074
Final R indexes [I>=2σ (I)]	$R_1= 0.0504$, w$R_2= 0.0963$
Final R indexes [all data]	$R_1= 0.0591$, w$R_2= 0.1011$
Largest diff. peak/hole / e Å^{-3}	1.28/-1.56

$R_1 = \Sigma\left\|F_o\right| - \left|F_c\right\|/\Sigma|F_o|$ and $wR_2 = \left[\Sigma w\left(F_o^2 - F_c^2\right)^2/\Sigma w\, F_o^4\right]^{1/2}$

Table S4. Atomic coordinates (x10^4), equivalent isotropic displacement parameters (Å^2×10^3) and BVS calculations for Sr$_2$Cd$_4$(B$_2$O$_5$)$_3$.

Atom	x	y	z	U(eq)	BVS
Sr(1)	2452.0(10)	8887.6(18)	3354.4(8)	16.5(3)	2.19
Cd(1)	4242.2(7)	4241.5 (13)	1333.7(6)	11.7(2)	1.92
Cd(2)	910.3(7)	4078.5(15)	1352.6(7)	21.3(3)	1.94
B(1)	3989(10)	4140(20)	4065(9)	12(2)	3.00
B(2)	2788(11)	-690(20)	878(10)	16(2)	2.98
B(3)	-520(11)	9020(20)	917(10)	19(2)	3.19
O(1)	3248(8)	5684(15)	4765(6)	27.1(19)	2.18
O(2)	4501(7)	5477(14)	3199(6)	17.3(15)	2.22
O(3)	5855(7)	6641(13)	704(5)	13.8(14)	1.80
O(4)	2644(7)	1460(13)	1523(6)	15.1(15)	2.01
O(5)	2493(7)	6975(13)	1300(6)	19.2(15)	2.05
O(6)	-831(10)	6587(19)	842(12)	61(4)	1.97
O(7)	40(20)	10690(30)	173(15)	38(5)	2.02
O(8)	684(11)	5630(20)	3204(9)	61(4)	1.91

Table S5. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $Sr_2Cd_4(B_2O_5)_3$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sr1	23.9(6)	12.4(5)	13.1(5)	2.5(3)	0.1(4)	-3.2(4)
Cd1	15.8(4)	9.9(4)	9.6(4)	-1.1(3)	2.9(2)	-0.5(3)
Cd2	19.0(4)	13.6(4)	30.9(5)	-1.5(3)	-6.2(3)	0.1(3)
B1	13(5)	15(6)	9(4)	3(4)	-1(4)	3(4)
B2	22(6)	9(5)	19(5)	0(4)	3(4)	-1(5)
B3	12(5)	22(6)	23(6)	3(5)	-4(4)	-2(5)
O1	44(5)	20(4)	18(4)	3(3)	11(3)	8(4)
O2	28(4)	16(4)	9(3)	0(3)	2(3)	-8(3)
O3	19(4)	14(3)	9(3)	1(2)	4(3)	0(3)
O4	18(4)	10(3)	18(3)	0(3)	2(3)	4(3)
O5	20(4)	12(4)	26(4)	4(3)	2(3)	1(3)
O6	32(6)	24(5)	124(11)	7(6)	-27(6)	-1(4)
O7	69(13)	23(11)	25(9)	-13(7)	30(9)	-21(10)
O8	58(7)	82(9)	41(6)	46(6)	-14(5)	-37(6)

Table S6. Selected bond lengths (Å) for $Sr_2Cd_4(B_2O_5)_3$.

$Sr_2Cd_4(B_2O_5)_3$			
Sr(1)-O(1)	2.472(8)	Cd(2)-O(5)	2.278(8)
Sr(1)-O(2)	2.841(8)	Cd(2)-O(6)	2.558(14)
Sr(1)-O(3)	2.530(7)	Cd(2)-O(6)	2.558(14)
Sr(1)-O(4)	2.526(7)	Cd(2)-O(7)	2.405(15)
Sr(1)-O(5)	2.579(8)	Cd(2)-O(8)	2.553(14)
Sr(1)-O(6)	2.449(11)	B(1)-O(1)	1.410(13)
Sr(1)-O(8)	2.552(10)	B(1)-O(2)	1.355(12)
Cd(1)-O(2)	2.258(7)	B(1)-O(3)	1.349(13)
Cd(1)-O(2)	2.440(7)	B(2)-O(1)	1.393(13)
Cd(1)-O(3)	2.398(6)	B(2)-O(4)	1.365(13)
Cd(1)-O(3)	2.277(7)	B(2)-O(5)	1.362(13)
Cd(1)-O(4)	2.265(7)	B(3)-O(6)	1.325(16)
Cd(1)-O(5)	2.357(7)	B(3)-O(7)	1.38(8)
Cd(2)-O(4)	2.310(7)	B(3)-O(8)	1.336(15)

Table S7. Selected bond angles (Å) for Sr$_2$Cd$_4$(B$_2$O$_5$)$_3$.

Sr$_2$Cd$_4$(B$_2$O$_5$)$_3$			
O(1)-Sr(1)-O(2)	50.6(2)	O(4)-Cd(1)-O(3)	88.0(2)
O(1)-Sr(1)-O(3)	83.3(3)	O(4)-Cd(1)-O(5)	78.1(2)
O(1)-Sr(1)-O(4)	151.7(2)	O(5)-Cd(1)-O(2)	158.0(3)
O(1)-Sr(1)-O(5)	108.9(2)	O(5)-Cd(1)-O(3)	95.6(3)
O(1)-Sr(1)-O(8)	79.8(3)	O(4)-Cd(2)-O(6)	90.0(3)
O(3)-Sr(1)-O(2)	81.2(2)	O(4)-Cd(2)-O(6)	170.2(4)
O(3)-Sr(1)-O(5)	125.6(2)	O(4)-Cd(2)-O(7)	95.7(3)
O(3)-Sr(1)-O(8)	158.3(3)	O(4)-Cd(2)-O(8)	104.1(3)
O(4)-Sr(1)-O(2)	101.4(2)	O(5)-Cd(2)-O(4)	78.8(3)
O(4)-Sr(1)-O(3)	88.6(2)	O(5)-Cd(2)-O(6)	96.36(19)
O(4)-Sr(1)-O(5)	55.5(2)	O(5)-Cd(2)-O(6)	93.6(3)
O(4)-Sr(1)-O(8)	112.7(3)	O(5)-Cd(2)-O(7)	138.5(4)
O(5)-Sr(1)-O(6)	69.9(2)	O(5)-Cd(2)-O(8)	83.8(3)
O(6)-Sr(1)-O(1)	112.1(4)	O(5)-Cd(2)-O(8)	169.0(3)
O(6)-Sr(1)-O(2)	161.4(3)	O(6)-Cd(2)-O(6)	80.3(5)
O(6)-Sr(1)-O(3)	90.6(3)	O(6)-Cd(2)-O(7)	89.4(6)
O(6)-Sr(1)-O(4)	95.1(3)	O(6)-Cd(2)-O(8)	85.4(3)
O(6)-Sr(1)-O(5)	127.7(3)	O(7)-Cd(2)-O(6)	48.7(5)
O(6)-Sr(1)-O(8)	83.2(4)	O(7)-Cd(2)-O(8)	48.9(4)
O(8)-Sr(1)-O(2)	98.2(3)	O(8)-Cd(2)-O(6)	96.0(3)
O(8)-Sr(1)-O(5)	73.4(3)	O(8)-Cd(2)-O(6)	85.7(5)
O(2)-Cd(1)-O(2)	88.58(18)	O(8)-Cd(2)-O(6)	164.9(4)
O(2)-Cd(1)-O(3)	172.7(2)	O(8)-Cd(2)-O(7)	137.2(5)
O(2)-Cd(1)-O(3)	94.5(2)	O(8)-Cd(2)-O(8)	88.3(3)
O(2)-Cd(1)-O(4)	99.2(2)	O(2)-B(1)-O(1)	112.1(9)
O(2)-Cd(1)-O(5)	84.8(3)	O(3)-B(1)-O(1)	121.0(9)
O(3)-Cd(1)-O(2)	93.6(2)	O(3)-B(1)-O(2)	126.9(9)
O(3)-Cd(1)-O(2)	95.9(3)	O(4)-B(2)-O(1)	123.6(9)
O(3)-Cd(1)-O(3)	78.4(3)	O(5)-B(2)-O(1)	115.2(9)
O(3)-Cd(1)-O(5)	105.5(3)	O(5)-B(2)-O(4)	121.2(9)
O(4)-Cd(1)-O(2)	82.3(2)	O(6)-B(3)-O(7)	133.4(13)
O(4)-Cd(1)-O(3)	166.2(2)	O(6)-B(3)-O(7)	98.3(12)

Symmetry transformations used to generate equivalent atoms:

[1]+X,1+Y,+Z; [2]1-X,1/2+Y,1/2-Z; [3]+X,1/2-Y,1/2+Z; [4]-X,-1/2+Y,1/2-Z; [5]-X,1/2+Y,1/2-Z; [6]1-X,-1/2+Y,1/2-Z; [7]+X,3/2-Y,-1/2+Z; [8]1-X,1-Y,-Z; [9]+X,-1+Y,+Z; [10]-X,1-Y,-Z; [11]+X,1/2-Y,-1/2+Z; [12]-X,2-Y,-Z

Figure S1. Experimental and calculated XRD patterns of compound of $Sr_2Cd_4(B_2O_5)_3$.
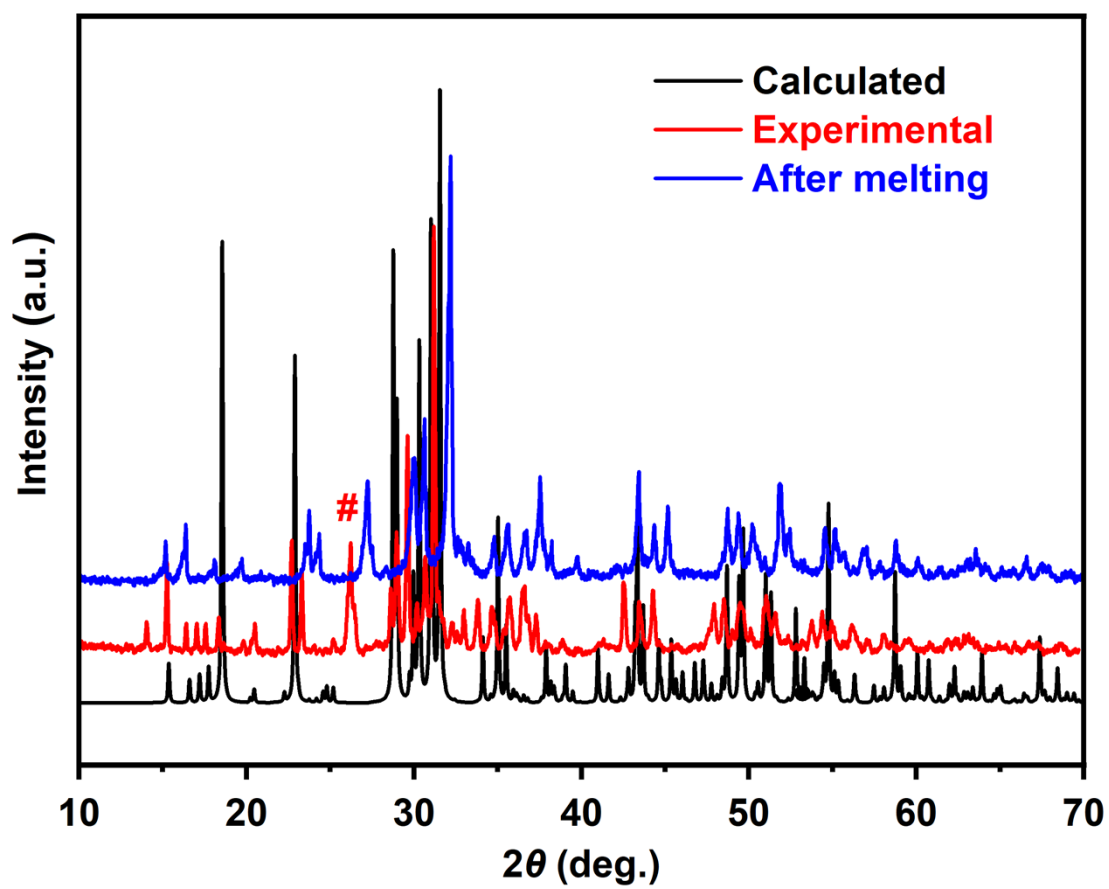
Figure S2. The isolated B_2O_5 with in α-SrCdB$_2$O$_5$(a), β-SrCdB$_2$O$_5$(b) and Sr$_2$Cd$_4$(B$_2$O$_5$)$_3$(c, d).

(a)

59.468 °

B(2) B(1)

(b)

42.713 °

B(1) B(2)

(c)

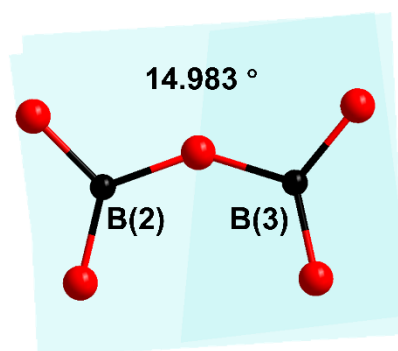0.000 °

B(1)   B(1)

(d)

14.983 °

B(2)   B(3)
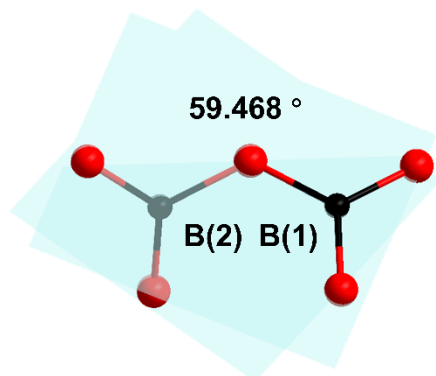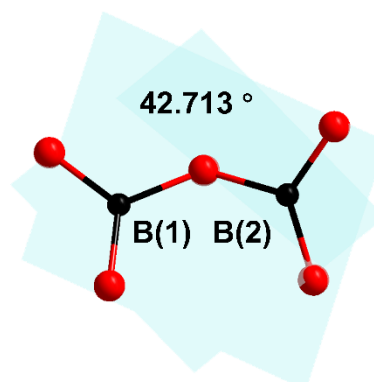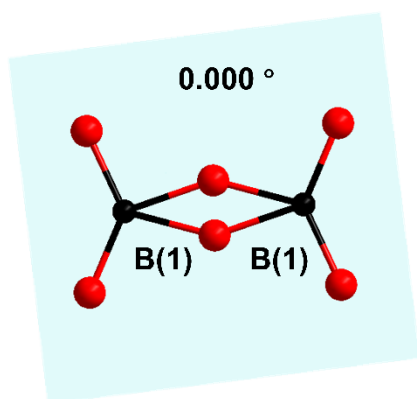
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