Supporting Information for

Two Bismuth Iodate Sulfates with Enhanced Optical Anisotropy

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Table S1. Crystallographic data of $Bi(IO_3)(SO_4)$ and $CdBi(IO_3)(SO_4)_2$.

formula	$Bi(IO_3)(SO_4)$	$CdBi(IO_3)(SO_4)_2$
formula weight	479.94	688.40
crystal system	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$
T (K)	293(2)	293(2)
a (Å)	9.4355(2)	12.777(2)
b (Å)	6.9168(2)	6.8491(9)
c (Å)	8.3374(2)	9.9835(14)
β (deg)	105.168(2)	103.226(15)
V (Å^3)	525.17(2)	850.5(2)
Z	4	4
D_c (g/cm^{-3})	6.070	5.376
μ (mm^{-1})	39.827	27.341
θ_{max}/deg	27.101	26.361
completeness/%	99.8	99.7
goodness of fit on F^2	1.115	1.018
R_1, wR_2 [I >2σ(I)][a]	0.0215, 0.0490	0.0299, 0.0500
R_1, wR_2 (all data)[a]	0.0223, 0.0493	0.0380, 0.0534
extinction coefficient	none	none

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$, and $wR_2 = \{\sum w[(F_o)^2 - (F_c)^2]^2/\sum w[(F_o)^2]^2\}^{1/2}$.

Table S2. Selected bond distances (Å) and the calculated bond orders of $Bi(IO_3)(SO_4)$ and $CdBi(IO_3)(SO_4)_2$.

$Bi(IO_3)(SO_4)$					
Bond	Bond length	Bond order	Bond	Bond length	Bond order
Bi(1)-O(2)#1	2.291(4)	0.59	Bi(1)-O(7)#6	2.727(5)	0.18
Bi(1)-O(6)#2	2.340(5)	0.51	I(1)-O(3)	1.808(5)	1.69
Bi(1)-O(1)#3	2.426(5)	0.41	I(1)-O(2)	1.816(4)	1.66
Bi(1)-O(4)#4	2.495(5)	0.34	I(1)-O(1)	1.839(4)	1.56
Bi(1)-O(5)	2.563(5)	0.28	S(1)-O(7)	1.467(5)	1.53
Bi(1)-O(4)	2.657(5)	0.22	S(1)-O(5)	1.477(5)	1.49
Bi(1)-O(1)	2.686(5)	0.20	S(1)-O(6)	1.477(5)	1.49
Bi(1)-O(5)#5	2.713(5)	0.19	S(1)-O(4)	1.495(5)	1.42
Symmetry transformations used to generate equivalent atoms:					
#1 -x+2, y-1/2, -z+5/2;		#2 -x+1, y-1/2, -z+3/2;		#3 x, -y+1/2, z-1/2;	
#4 -x+1, -y, -z+2;		#5 x, -y+1/2, z+1/2;		#6 -x+1, y+1/2, -z+3/2.	
$CdBi(IO_3)(SO_4)_2$					
Bond	Bond length	Bond order	Bond	Bond length	Bond order
Cd(1)-O(8)	2.217(6)	0.43	I(1)-O(2)	1.771(6)	1.87
Cd(1)-O(7)	2.232(5)	0.41	I(1)-O(1)	1.856(5)	1.49
Cd(1)-O(9)#1	2.247(6)	0.40	I(1)-O(3)	1.976(5)	1.07
Cd(1)-O(6)#2	2.275(6)	0.37	I(1)-O(3)#6	2.085(5)	0.80
Cd(1)-O(4)#3	2.313(5)	0.33	S(1)-O(7)	1.454(6)	1.58
Cd(1)-O(4)#4	2.358(5)	0.29	S(1)-O(6)	1.472(6)	1.51
Bi(1)-O(1)	2.236(5)	0.68	S(1)-O(5)	1.478(7)	1.48
Bi(1)-O(2)#5	2.255(6)	0.65	S(1)-O(4)	1.486(5)	1.45

Bi(1)-O(3)#6	2.314(5)	0.55	S(2)-O(8)	1.458(6)	1.57
Bi(1)-O(5)	2.460(6)	0.37	S(2)-O(9)	1.470(6)	1.52
Bi(1)-O(11)#1	2.554(5)	0.29	S(2)-O(11)	1.471(6)	1.51
Bi(1)-O(10)#5	2.603(6)	0.25	S(2)-O(10)	1.477(6)	1.49

Symmetry transformations used to generate equivalent atoms:

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

#4 x, y+1, z; #5 x, -y+1/2, z+1/2; #6 -x+1, y+1/2, -z+1/2.

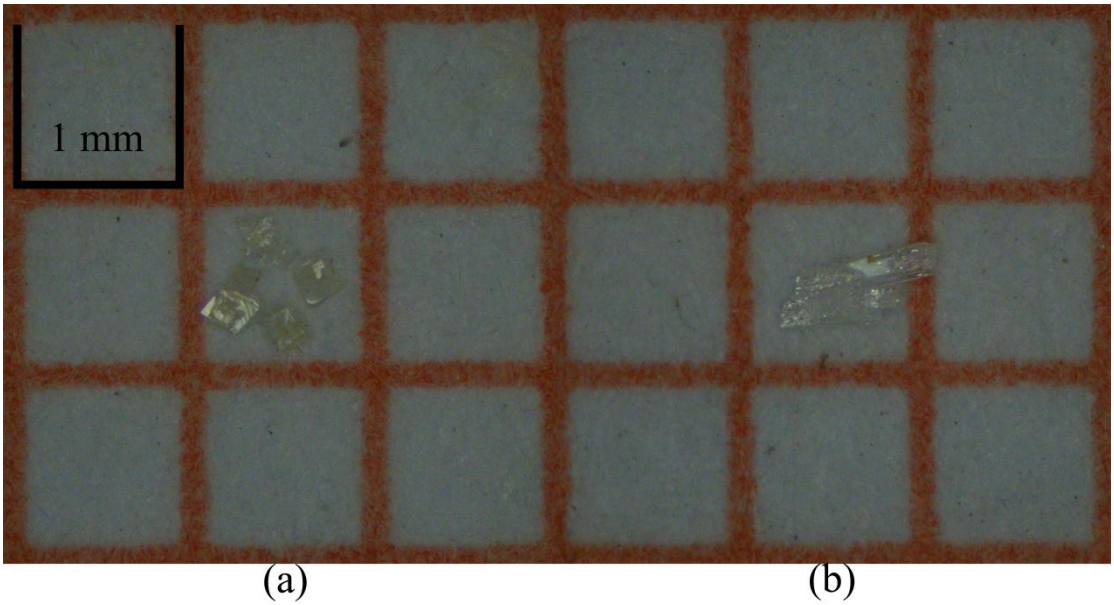

Figure S1. The photographs of $Bi(IO_3)(SO_4)$ (a) and $CdBi(IO_3)(SO_4)_2$ (b)

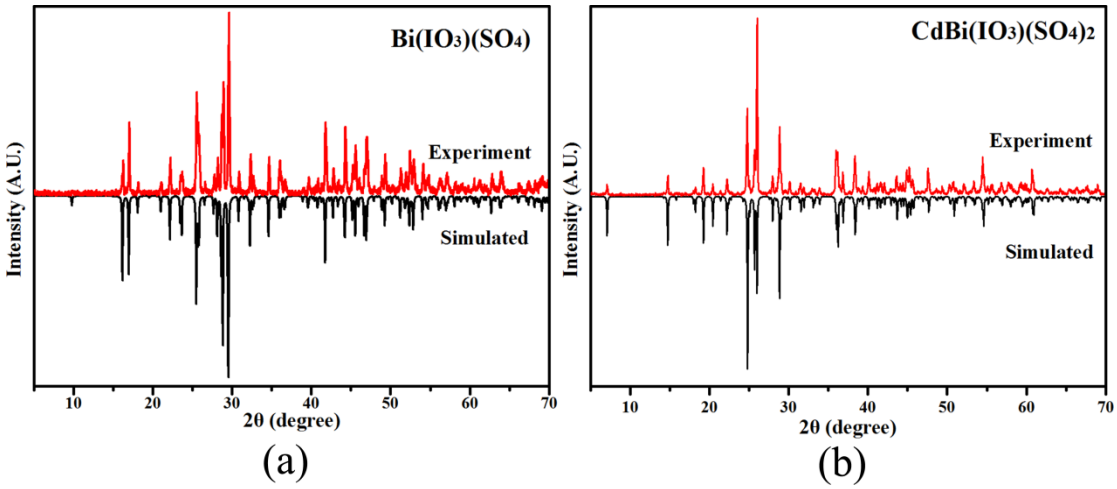

Figure S2. Experimental and simulated powder X-ray diffraction (PXRD) patterns of $Bi(IO_3)(SO_4)$ (a) and $CdBi(IO_3)(SO_4)_2$ (b).

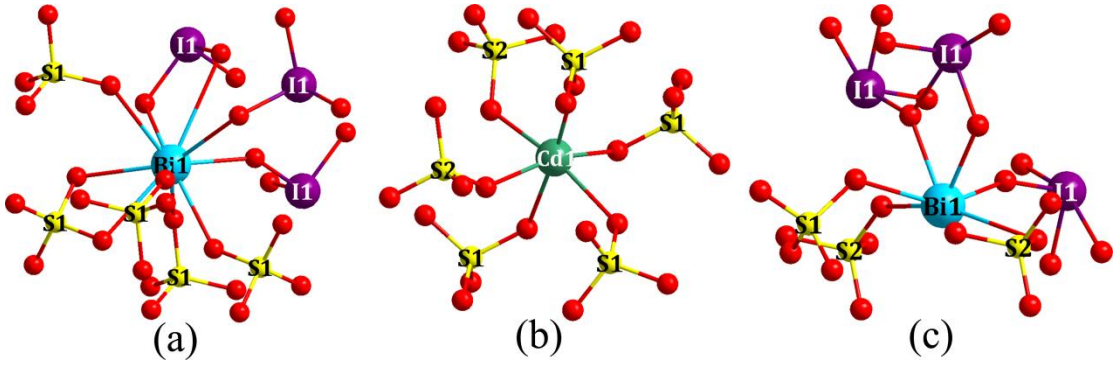

Figure S3. View of the coordination geometry around Bi^{3+} (a) in $Bi(IO_3)(SO_4)$ and the coordination geometries around Cd^{2+} (b) and Bi^{3+} (c) in $CdBi(IO_3)(SO_4)_2$.

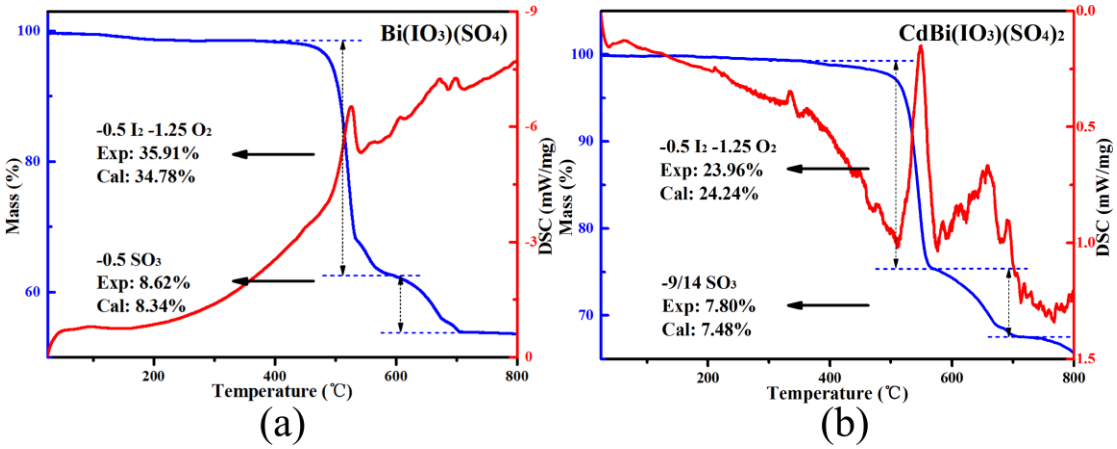

Figure S4. Thermogravimetry (TG) and differential scanning calorimetry (DSC) curves of $Bi(IO_3)(SO_4)$ (a) and $CdBi(IO_3)(SO_4)_2$ (b).

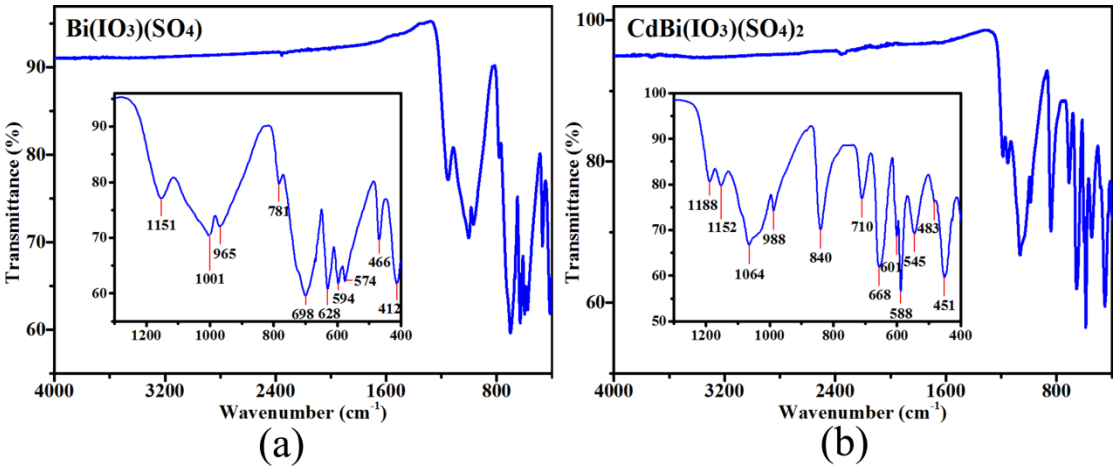

Figure S5. Infrared spectra of $Bi(IO_3)(SO_4)$ (a) and $CdBi(IO_3)(SO_4)_2$ (b).

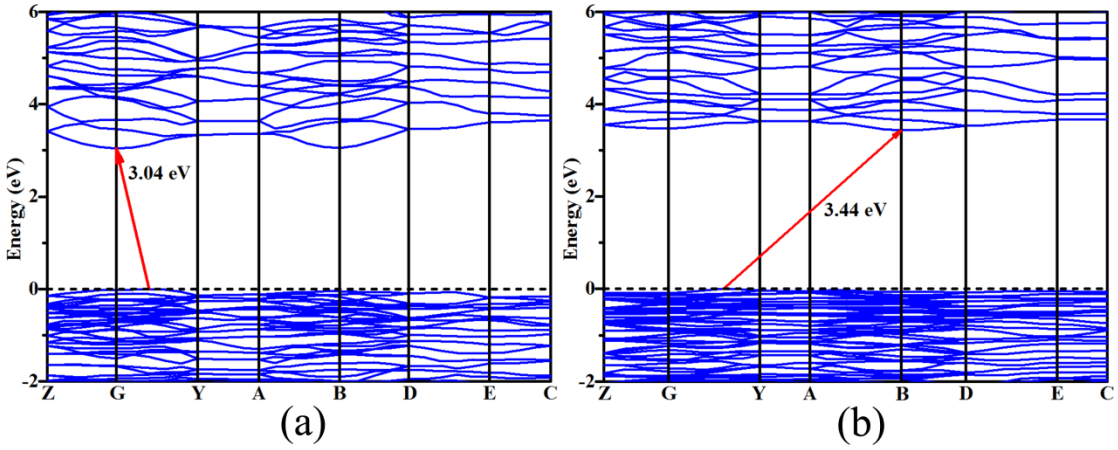

Figure S6. Calculated band structures of $Bi(IO_3)(SO_4)$ (a) and $CdBi(IO_3)(SO_4)_2$ (b).

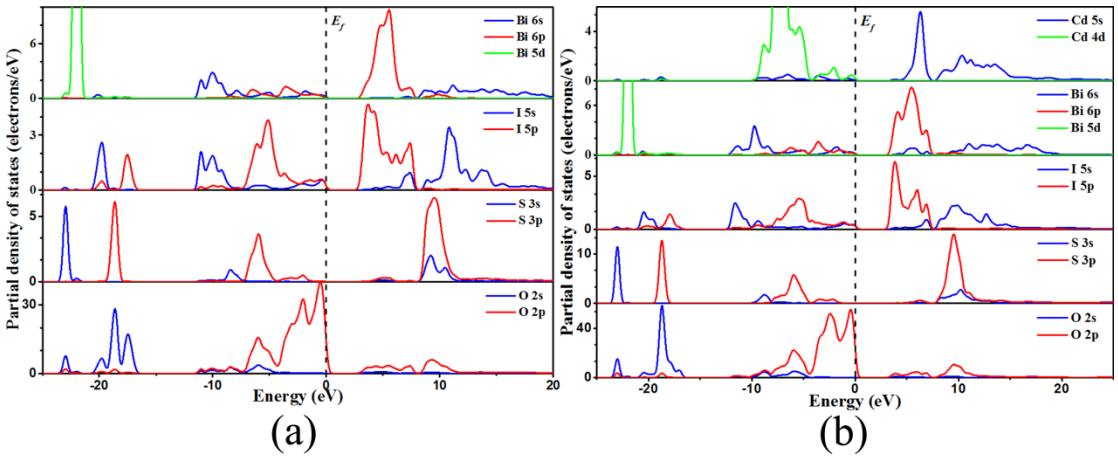

Figure S7. Partial density of states of $Bi(IO_3)(SO_4)$ (a) and $CdBi(IO_3)(SO_4)_2$ (b).