From BiF_3 to $BiF_3 \cdot H_2O$: Diverse Bi(Ⅲ) Coordination for Structural transformation and Birefringence Regulation

Xian Liu [a], Can Yang [a], Qi Wu [a*], Juan Sun [a], Fei Liang [b*]

a. College of Chemistry and Chemical Engineering, Hubei Normal University, Huangshi 435002, P. R. China.

b. State key Laboratory of crystal Materials and Institute of Crystal Materials, Shandong University, Jinan 250100, P. R. China.

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Table S1. Selected bond lengths (Å) for $BiF_3 \cdot H_2O$

bond	lengths (Å)	bond	lengths (Å)
Bi1-F1[3]	2.456(6)	Bi1-F1[7]	2.456(6)
Bi1-F1[4]	2.409(3)	Bi1-F1[8]	2.456(6)
Bi1-F1[5]	2.456(6)	Bi1-F1[9]	2.456(6)
Bi1-F1[6]	2.409(3)	Bi1-F1[10]	2.456(6)
Bi1-F1	2.409(3)		

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

Table S2. Selected bond angles (°) for $BiF_3 \cdot H_2O$

bond	angles (°)	bond	angles (°)
F1[4]-Bi1-F1[7]	69.9(3)	F1-Bi1-F1[6]	69.9(3)
F1[3]-Bi1-F1[9]	69.6(3)	F1[7]-Bi1-F1[3]	141.54(13)
F1[7]-Bi1-F1[9]	141.53(13)	F1[10]-Bi1-F1[6]	141.53(13)
F1[10]-Bi1-F1[7]	97.6(3)	F1[10]-Bi1-F1[3]	69.6(3)
F1[10]-Bi1-F1[9]	69.6(3)	F1[7]-Bi1-F1[6]	69.6(3)
F1[4]-Bi1-F18	131.19(17)	F1[5]-Bi1-F1[8]	69.9(3)
F1[5]-Bi1-F1	120.001(2)	F1[8]-Bi1-F1[6]	69.6(3)
F1[5]-Bi1-$F1_4$	119.999(1)	F1[8]-Bi1-F1[3]	97.6(3)
F1[5]-Bi1-F1[6]	131.19(16)	F1[3]-Bi1-F1[6]	141.53(13)
F1[5]-Bi1-F1[3]	69.9(3)	F1[5]-Bi1-F1[7]	71.6(3)
F1-Bi1-F1[8]	71.6(3)	F1[9]-Bi1-F1[6]	97.6(3)

$F1^4$-Bi1-$F1^3$	131.19(17)	$F1^5$-Bi1-$F1^9$	131.19(16)
$F1^4$-Bi1-F1	120.000(2)	$F1^{10}$-Bi1-$F1^8$	141.54(13)
$F1^5$-Bi1-$F1^{10}$	71.6(3)	$F1^7$-Bi1-F18	69.6(3)
$F1^8$-Bi1-$F1^9$	141.53(13)	$F1^4$-Bi1-$F1^6$	71.6(3)
F1-Bi1-F110	131.19(16)	F14-Bi1-F19	71.6(3)
F14-Bi1-F110	69.9(3)	F1-Bi1-F17	131.19(16)
F1-Bi1-F19	69.9(3)		

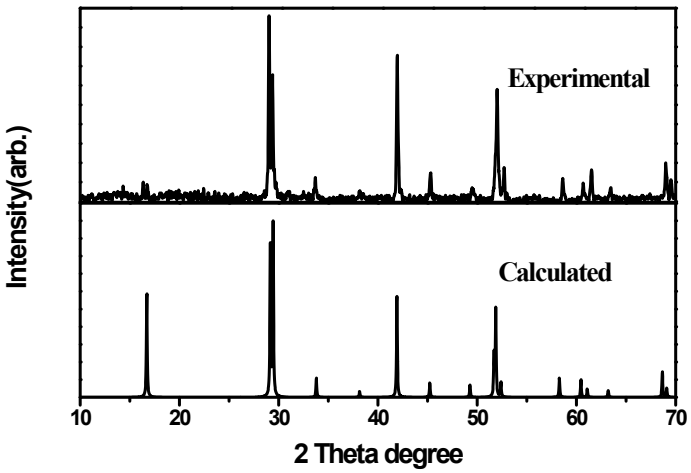

Fig. S1 Simulated and measured powder X-ray diffraction patterns of $BiF_3 \cdot H_2O$

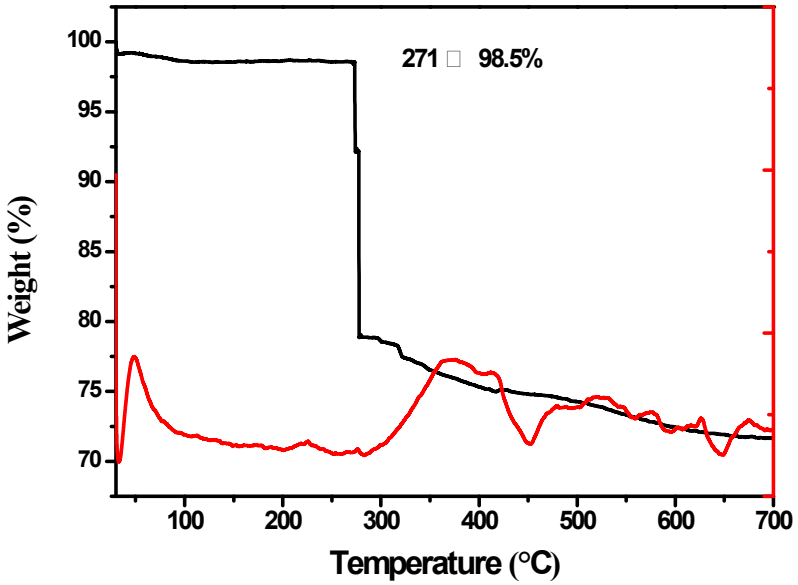

Fig. S2 The TGA and DSC of $BiF_3 \cdot H_2O$

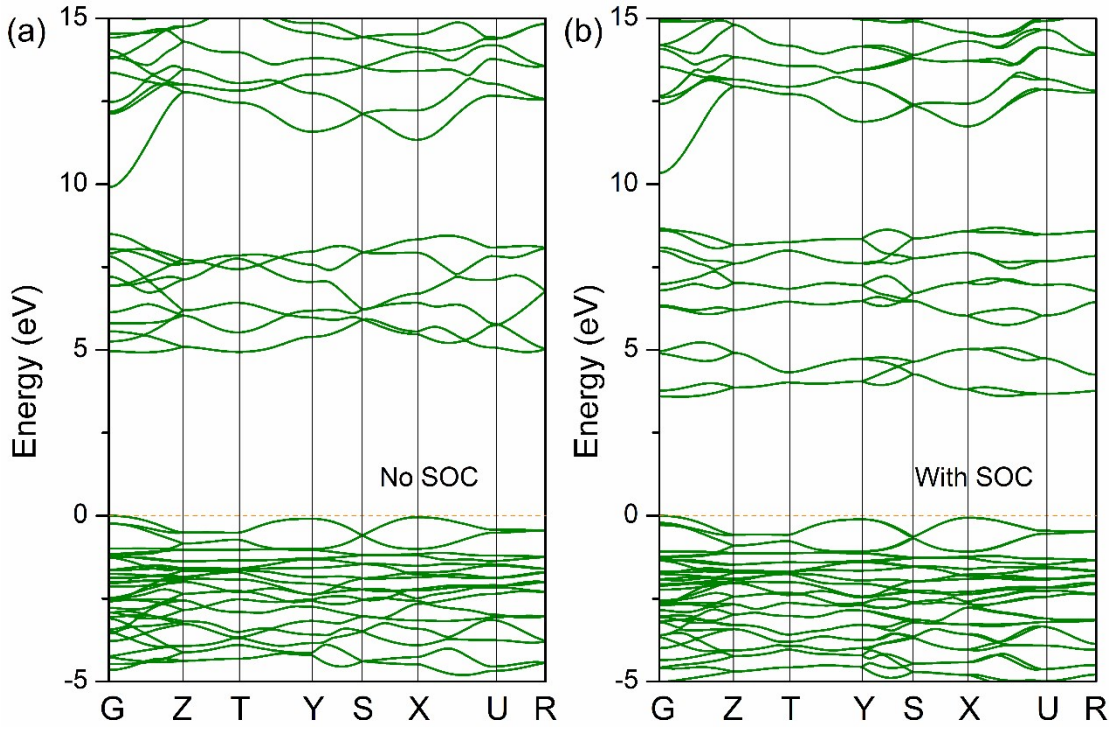

Fig. S3 Calculated band structure by PBE functional of orthogonal BiF_3, (a) without spin-orbital coupling and (b) with spin-orbital coupling.

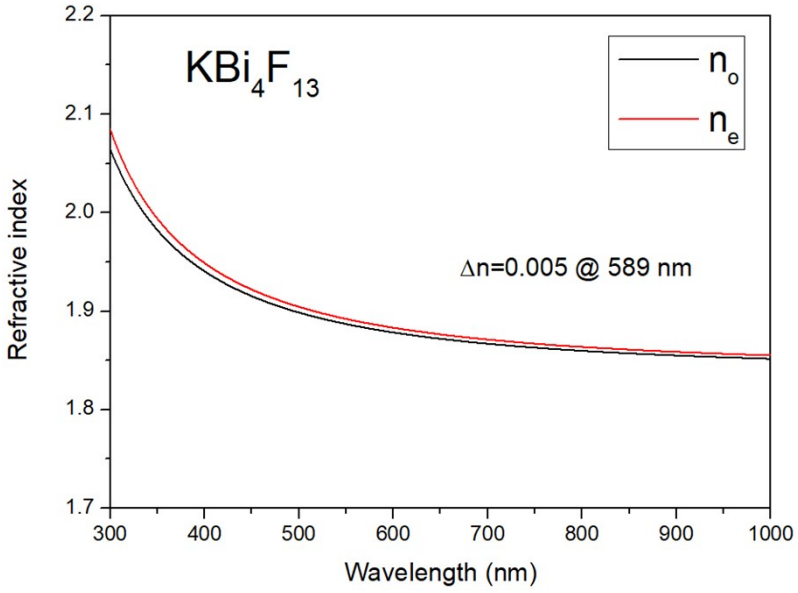

Fig. S4 The simulated refractive index of KBi_4F_{13}