$Ba_{18}F_{18}In_8S_{21}$ and $Ba_9F_{10}In_4S_{10}$: New kind of Mixed Anions Compounds with the Novel Low-Dimensional Structure

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Electronic Supplementary Information

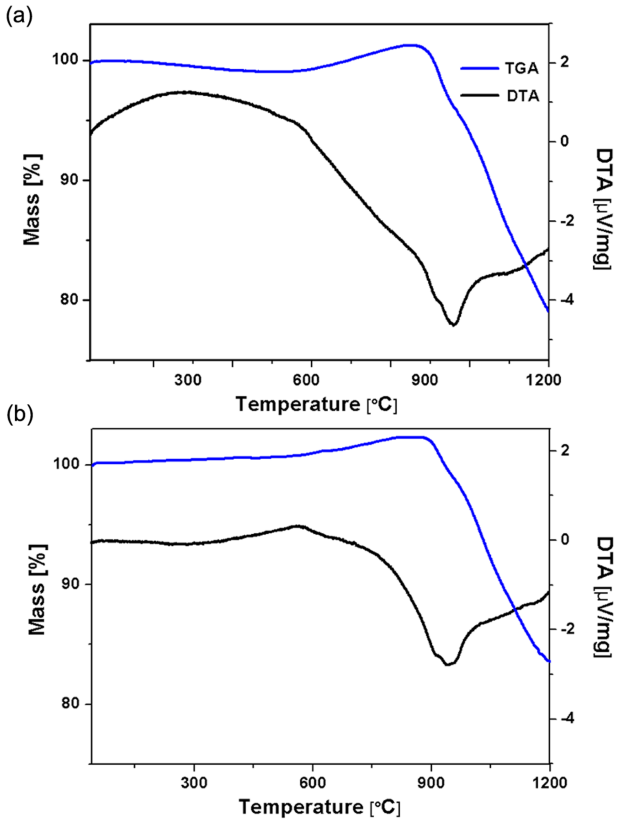

Fig. S1 TGA and DTA diagrams of **1** (a) and **2** (b).

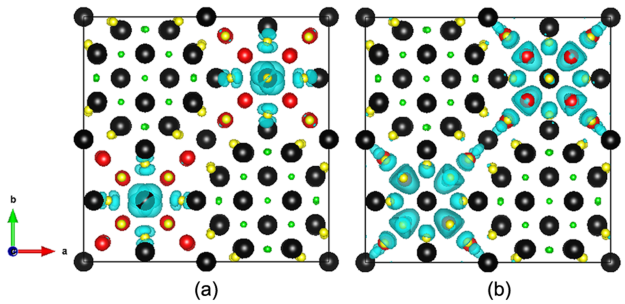

Fig. S2 The isosurfaces (iso-value = 0.00034 e/Å^3) of charge distribution at the G point of HVB (a) and LCB (b) of **1**. Black, Ba; red, In; yellow, S; green, F.

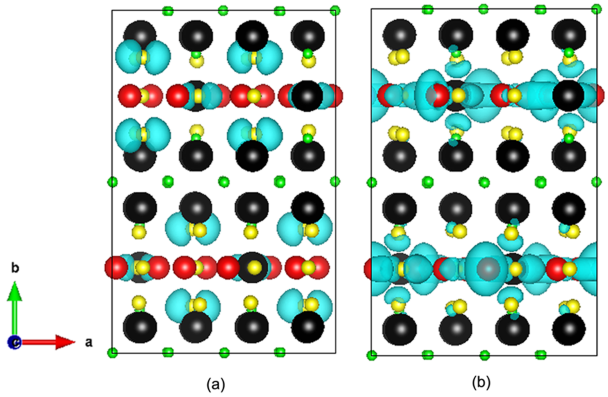

Fig. S3 The isosurfaces (iso-value = 0.00053 e/Å^3) of charge distribution at the G point of HVB (a) and LCB (b) of **2**. Black, Ba; red, In; yellow, S; green, F.

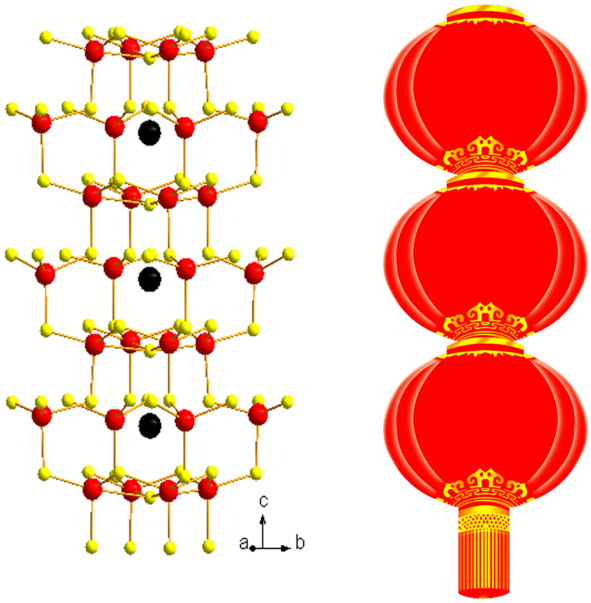

Fig. S4 The 1D [$BaIn_8S_{21}$] covalent region looks like a string of red lanterns in **1**. Black, Ba; red, In; yellow, S.

Table S1. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) of **1** and **2**.

Atom	*x*	*y*	*z*	U_{eq} [a]
		$Ba_{18}F_{18}In_8S_{21}$		
Ba(1)	0.1549(1)	0.5548(1)	0.1308(1)	0.010(1)
Ba(2)	0.3522(1)	0.5539(1)	0.1246(1)	0.009(1)
Ba(3)	0.6503(1)	0.2502(1)	0.3760(1)	0.009(1)
Ba(4)	0.2497(1)	0.0406(1)	0.3799(1)	0.010(1)
Ba(5)	0	0	0.5000	0.054(1)
Ba(6)	0.2500	0.2500	0.2952(1)	0.017(1)
In(1)	0.1604(1)	0.1604(1)	0.0737(1)	0.017(1)
In(2)	0.0744(1)	0.0744(1)	-0.1677(1)	0.012(1)
In(3)	0.0805(1)	0.0805(1)	0.3144(1)	0.012(1)

In(4)	0.3435(1)	0.1565(1)	0.0795(1)	0.018(1)
S(1)	0.0819(1)	0.0819(1)	0.1217(3)	0.014(1)
S(2)	0.0779(1)	0.0779(1)	-0.3684(3)	0.015(1)
S(3)	0.1542(1)	0.1542(1)	-0.1222(3)	0.011(1)
S(4)	0.1552(1)	0.1552(1)	0.3824(3)	0.011(1)
S(5)	0.2510(1)	0.1005(2)	0.1361(2)	0.024(1)
S(6)	0.2500	0.2500	0.0506(6)	0.035(2)
S(7)	-0.0183(1)	0.1112(1)	0.3801(2)	0.014(1)
S(8)	-0.0201(1)	0.1202(1)	-0.1238(2)	0.011(1)
F(1)	0.2500	0.7500	0.2500	0.016(3)
F(2)	0.6525(3)	0.1525(3)	0.5000	0.014(2)
F(3)	0.2544(2)	0.5511(3)	0.2464(5)	0.013(1)
F(4)	0.2507(2)	0.5521(3)	0.0088(5)	0.014(1)
F(5)	0.1521(3)	0.6521(3)	0	0.014(2)
F(6)	0.6528(3)	0.1534(3)	0.2501(4)	0.014(1)
F(7)	0.2500	0.7500	0	0.015(3)
		$Ba_9F_{10}In_4S_{10}$		
Ba(1)	0.3689(1)	0.5759(1)	0.2563(1)	0.012(1)
Ba(2)	0.1219(1)	0.5774(1)	0.0037(1)	0.012(1)
Ba(3)	0.1188(1)	0.4243(1)	0.2501(1)	0.012(1)
Ba(4)	0.6284(1)	0.5753(1)	-0.0057(1)	0.012(1)
Ba(5)	-0.1269(1)	0.7500	-0.0008(1)	0.035(1)
In(1)	0.1757(1)	0.7500	0.1973(1)	0.019(1)
In(2)	0.0801(1)	0.7500	-0.2953(1)	0.019(1)
In(3)	0.2940(1)	0.7500	-0.0834(1)	0.048(1)
In(4)	0.4811(1)	0.7500	0.1056(1)	0.054(1)
S(1)	0.3622(3)	0.7500	0.2595(3)	0.017(1)
S(2)	0.1072(2)	0.6419(2)	0.2663(2)	0.023(1)
S(3)	0.3798(2)	0.6476(2)	0.0057(2)	0.025(1)
S(4)	0.1389(2)	0.6376(2)	-0.2377(2)	0.024(1)
S(5)	0.1351(3)	0.7500	-0.4875(3)	0.017(1)

S(6)	0.1217(3)	0.7500	0.0075(3)	0.017(1)
S(7)	0.3858(3)	0.7500	-0.2544(3)	0.019(1)
F(1)	-0.1242(4)	0.6265(3)	-0.0014(4)	0.017(2)
F(2)	0.5030(4)	0.4983(3)	-0.1244(5)	0.013(1)
F(3)	0.4971(4)	0.5003(3)	0.3763(5)	0.015(2)
F(4)	0.7463(4)	0.4974(3)	0.1203(5)	0.014(1)
F(5)	0.2458(4)	0.5026(3)	0.1297(5)	0.015(1)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond-valence sums, bond lengths (Å) and angles (deg) of **1** and **2**.

	distance	BV		distance	BV
			$Ba_{18}F_{18}In_8S_{21}$		
Ba(1)-F(4)	2.616(6)	0.3162	Ba(6)-S(6)	3.086(7)	0.4256
Ba(1)-F(6)#1	2.634(6)	0.3012	Ba(6)-S(4)#11	3.158(3)	0.3504
Ba(1)-F(3)	2.636(6)	0.2995	Ba(6)-S(4)	3.158(3)	0.3504
Ba(1)-F(5)	2.709(4)	0.2459	Ba(6)-S(3)#19	3.167(3)	0.3420
Ba(1)-S(7)#2	3.265(3)	0.2624	Ba(6)-S(3)#3	3.167(3)	0.3420
Ba(1)-S(8)#3	3.280(2)	0.2519	Ba(6)-S(6)#19	3.221(7)	0.2955
Ba(1)-S(2)#3	3.3869(11)	0.1887		∑BVS=	2.1095
Ba(1)-S(7)#4	3.403(3)	0.1807	In(1)-S(3)	2.479(4)	0.7249
	∑BVS=	2.0465	In(1)-S(5)	2.523(3)	0.6436
Ba(3)-F(6)	2.663(6)	0.2785	In(1)-S(5)#1	2.523(3)	0.6436
Ba(3)-F(5)#3	2.665(5)	0.2770	In(1)-S(1)	2.527(4)	0.6367
Ba(3)-F(2)	2.665(4)	0.2770	In(1)-S(6)	2.8105(13)	0.2959
Ba(3)-F(6)#14	2.669(6)	0.2740		∑BVS=	2.9447
Ba(3)-F(7)#15	2.699(6)	0.2740	In(2)-S(8)#1	2.383(2)	0.9397
Ba(3)-F(1)#16	2.7135(6)	0.2429	In(2)-S(8)	2.383(2)	0.9397
Ba(3)-F(3)#1	2.735(6)	0.2292	In(2)-S(2)	2.534(4)	0.6248
Ba(3)-F(4)#3	2.740(6)	0.2261	In(2)-S(3)	2.554(4)	0.6248
	∑BVS=	2.0787		∑BVS=	3.129
Ba(4)-F(4)#18	2.613(6)	0.3188	F(4)-Ba(1)-F(6)#1	111.4(2)	
Ba(4)-F(3)#11	2.633(6)	0.3020	F(4)-Ba(1)-F(3)	69.63(19)	

Ba(4)-S(8)#19	3.169(2)	0.3401	F(5)-Ba(1)-S(7)#2	69.54(11)	
Ba(4)-S(4)	3.279(3)	0.2527	S(7)#2-Ba(1)-S(8)#3	85.02(6)	
Ba(4)-S(3)#19	3.284(3)	0.2493	F(3)-Ba(1)-S(2)#3	112.90(15)	
Ba(4)-S(7)#1	3.321(3)	0.2255	S(3)-In(1)-S(1)	99.34(12)	
Ba(4)-S(5)	3.348(3)	0.2097	S(8)#1-In(2)-S(2)	104.25(7)	
Ba(4)-S(5)#20	3.492(3)	0.1421	S(2)-In(2)-S(3)	100.49(12)	
	∑BVS=	2.0402	S(7)-In(3)-S(4)	107.01(8)	
			$Ba_9F_{10}In_4S_{10}$		
Ba(1)-F(5)	2.631(6)	0.3036	In(1)-S(2)#9	2.417(3)	0.8572
Ba(1)-F(3)	2.647(6)	0.2908	In(1)-S(2)	2.417(3)	0.8572
Ba(1)-F(4)#1	2.660(6)	0.2807	In(1)-S(1)	2.471(4)	0.7408
Ba(1)-F(2)#2	2.718(6)	0.2400	In(1)-S(6)	2.483(4)	0.7172
Ba(1)-F(1)#3	3.237(6)	0.0590		∑BVS=	3.1724
Ba(1)-S(2)#3	3.267(3)	0.2610	In(3)-S(7)	2.442(4)	0.8254
Ba(1)-S(1)	3.3591(7)	0.2034	In(3)-S(6)	2.449(4)	0.8143
Ba(1)-S(3)	3.446(3)	0.1609	In(3)-S(3)#9	2.514(3)	0.6776
Ba(1)-S(2)	3.529(3)	0.1285	In(3)-S(3)	2.514(3)	0.6776
	∑BVS=	1.9279		∑BVS=	2.994
Ba(4)-F(2)	2.631(6)	0.3036	F(5)-Ba(1)-F(3)	114.05(17)	
Ba(4)-F(4)	2.640(6)	0.2963	F(3)-Ba(1)-F(4)#1	72.89(16)	
Ba(4)-F(5)#2	2.682(6)	0.2645	S(3)-Ba(1)-S(2)	85.71(7)	
Ba(4)-F(2)#2	2.724(6)	0.2362	S(4)-Ba(2)-S(3)	79.01(8)	
Ba(4)-F(1)#7	3.262(6)	0.0552	F(4)#1-Ba(3)-S(4)#6	66.91(13)	
Ba(4)-S(2)#3	3.285(3)	0.2486	S(2)-In(1)-S(6)	104.36(9)	
Ba(4)-S(5)#8	3.3701(7)	0.1976	S(4)#9-In(2)-S(5)	101.85(8)	
Ba(4)-S(3)	3.424(3)	0.1707	S(6)-In(3)-S(3)	99.85(9)	
Ba(4)-S(4)#8	3.448(3)	0.1600	S(5)#8-In(4)-S(1)	165.14(16)	
	∑BVS=	1.9327	S(1)-In(4)-S(3)	94.69(9)	

Symmetry transformations used to generate equivalent atoms:

For $Ba_{18}F_{18}In_8S_{21}$: #1 y,x,z #2 -x,y+1/2,-z+1/2 #3 y,-x+1/2,z+1/2 #4 y,-x+1/2,z-1/2 #11 -x+1/2,-y+1/2,z #14 y+1/2,-x+1,-z+1/2 #15 -y+3/2,x,z+1/2 #16 x+1/2,-y+1,-z+1/2 #18 x,-y+1/2,z+1/2 #19 -y+1/2,x,z+1/2 #20 -x+1/2,y,z+1/2

For $Ba_9F_{10}In_4S_{10}$: #1 x-1/2,y,-z+1/2 #2 -x+1,-y+1,-z #3 x+1/2,y,-z+1/ #6 -x+1/2,-y+1,z+1/2 #7 x+1,y,z #8 x+1/2,y,-z-1/2 #9 x,-y+3/2,z