Electronic Supplementary Material (ESI) for CrystEngComm

Syntheses, Crystal and Electronic Structures, and Characterizations of the Mixed Anions Compounds $Ba_4In_2Te_2Q_5$ (Q = S, Se)

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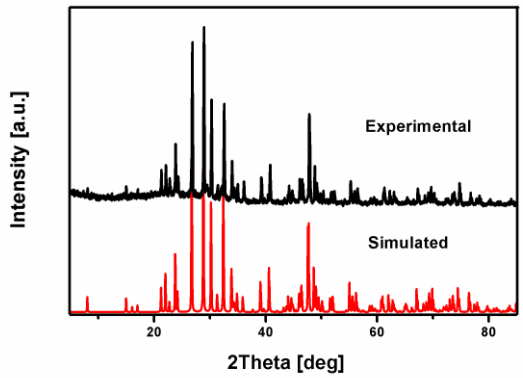
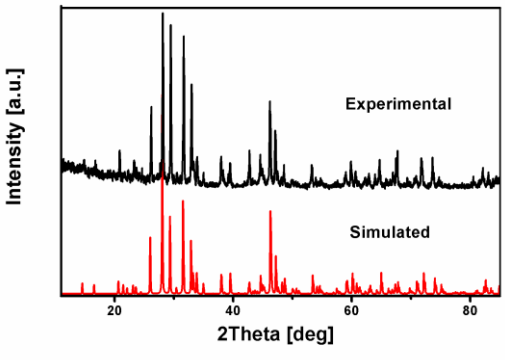
Electronic Supplementary Information

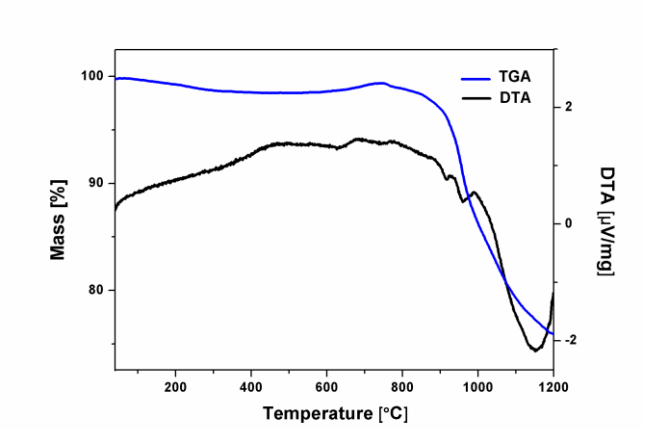


(a)

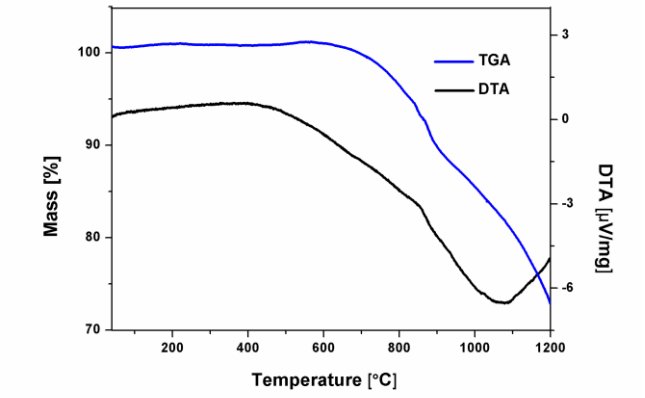


(b)

Fig. S1 Experimental and simulated X-ray diffraction patterns for polycrystalline **1** (a) and **2** (b). (The radiation wavelength of the X-ray is λ = 1.5418 Å).



(a)



(b)

Fig. S2 TGA and DTA diagrams of **1** (a) and **2** (b), the measurement results indicate that the two compounds are thermally stable up to high temperature.

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

Atom	*x*	*y*	*z*	$U_{eq}{}^a$
		$Ba_4In_2Te_2S_5$		
Ba(1)	0.6586(1)	0.1586(1)	0	0.012(1)
Ba(2)	1.0000	0	0.2822(1)	0.014(1)

In(1)	0.5000	0	0.3399(1	0.012(1)
Te(1)	0.6840(1)	0.1840(1)	0.5000	0.014(1)
S(1)	0.3438(2)	0.1562(2)	0.1959(2)	0.014(1)
S(2)	1.0000	0	0	0.011(1)
		$Ba_4In_2Te_2Se_5$		
Ba(1)	0.6560(1)	0.1560(1)	0	0.012(1)
Ba(2)	1.0000	0	0.2879(1)	0.016(1)
In(1)	0.5000	0	0.3459(1)	0.013(1)
Te(1)	0.6794(1)	0.1795(1)	0.5000	0.018(1)
Se(1)	0.3412(1)	0.1588(1)	0.1991(1)	0.014(1)
Se(2)	1.0000	0	0	0.012(1)

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

Table S2 Selected bond lengths (Å), bond angles (deg) for compounds **1** and **2**.

		$Ba_4In_2Te_2S_5$	
Ba(1)-S(1)#1	3.079(2)	Ba(2)-Te(1)	3.8913(5)
Ba(1)-S(1)#2	3.079(2)	In(1)-S(1)	2.4379(19)
Ba(2)-Te(1)#11	3.8913(5)	In(1)-S(1)#6	2.4379(19)
Ba(2)-Te(1)#12	3.8913(5)	In(1)-Te(1)	2.8041(8)
S(1)#1-Ba(1)-S(1)#2	89.23(8)	S(1)-In(1)-S(1)#6	98.60(10)
S(2)-Ba(2)-Te(1)	128.162(9)	S(1)-In(1)-Te(1)	114.27(3)
Te(1)#11-Ba(2)-Te(1)	67.556(9)	In(1)-S(1)-Ba(1)	90.15(5)
		$Ba_4In_2Te_2Se_5$	
Ba(1)-Se(1)#1	3.1849(12)	Ba(2)-Te(1)	3.9669(6)
Ba(1)-Se(1)#2	3.1849(11)	In(1)-Se(1)	2.5467(11)
Ba(2)-Te(1)#11	3.9669(6)	In(1)-Se(1)#6	2.5467(11)
Ba(2)-Te(1)#12	3.9669(6)	In(1)-Te(1)	2.7932(9)

Se(1)#1-Ba(1)-Se(2)	75.573(13)	Se(1)-In(1)-Se(1)#6	98.67(5)
Se(1)#2-Ba(1)-Se(2)	75.573(13)	Se(1)-In(1)-Te(1)	113.985(13)
Se(2)-Ba(2)-Te(1)#12	127.192(10)	In(1)-Te(1)-Ba(2)#12	123.104(18)

Symmetry transformations used to generate equivalent atoms:

#1 -y+1, x, z #2 -y+1, x, -z #6 -x+1, -y, z

#11 y+1, -x+1, -z+1 #12 -x+2, -y, -z+1

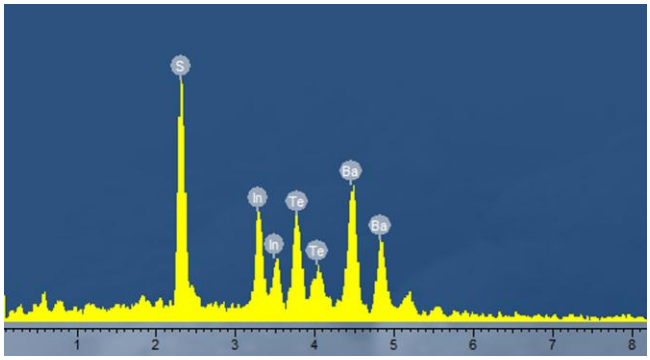


Fig. S2 EDX spectrum of $Ba_4In_2Te_2S_5$ single crystal.

Point 1				**Point 2**			
Element	*Weight%*	*Atomic%*	*Formula*	*Element*	*Weight%*	*Atomic%*	*Formula*
S K	13.30	38.17	5.10	S K	13.59	38.75	5.37
In L	20.59	16.50	2.20	In L	20.65	16.45	2.28
Te L	20.75	14.96	2.00	Te L	20.14	14.43	2.00
Ba L	45.35	30.38	4.06	Ba L	45.62	30.37	4.20
Totals	100.00			Totals	100.00		
Point 3				**Point 4**			
Element	*Weight%*	*Atomic%*	*Formula*	*Element*	*Weight%*	*Atomic%*	*Formula*
S K	12.59	36.63	4.70	S K	13.74	39.07	5.74
In L	21.67	17.61	2.25	In L	20.80	16.52	2.42

Te L	21.31	15.58	2.00	Te L	19.03	13.60	2.00
Ba L	44.43	30.18	3.87	Ba L	46.43	30.82	4.53
Totals	100.00			Totals	100.00		

Point 5

Element	*Weight%*	*Atomic%*	*Formula*	
S K	12.96	37.42	5.69	
In L	22.69	18.29	2.78	Average formula: $Ba_{4.2(7)}In_{2.3(8)}Te_2S_{5.3(2)}$
Te L	18.13	13.15	2.00	
Ba L	46.21	31.14	4.73	
Totals	100.00			

Point 1

Element	*Weight%*	*Atomic%*	*Formula*
Se L	32.05	43.54	5.60
In L	16.62	15.53	2.00
Te L	14.41	12.11	1.56
Ba L	36.92	28.83	3.71
Totals	100.00		

Point 2

Element	*Weight%*	*Atomic%*	*Formula*
Se L	31.13	42.47	5.15
In L	17.55	16.47	2.00
Te L	13.49	11.39	1.38
Ba L	37.83	29.67	3.60
Totals	100.00		

Point 3

Element	*Weight%*	*Atomic%*	*Formula*
Se L	31.43	42.47	5.15
In L	17.55	16.47	2.00
Te L	13.49	11.39	1.38
Ba L	37.83	29.67	3.60
Totals	100.00		

Point 4

Element	*Weight%*	*Atomic%*	*Formula*
Se L	31.00	42.37	5.70
In L	15.82	14.87	2.00
Te L	15.97	13.51	1.82
Ba L	37.21	29.25	3.93
Totals	100.00		

Point 5				
Element	*Weight%*	*Atomic%*	*Formula*	
Se L	31.00	42.37	5.70	
In L	15.82	14.87	2.00	Average formula: $Ba_{3.7(5)}In_2Te_{1.6(2)}Se_{5.4(6)}$
Te L	15.97	13.51	1.82	
Ba L	37.21	29.25	3.93	
Totals	100.00			