Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthesis and Characterization of a New Mid-Infrared Transparency Compound: Acentric $Ba_5In_4Te_4S_7$

De-Ming Tan[a,b], Chen-Sheng Lin[a], Zhong-Zhen Luo[a], Hao Zhang[a], Wei-Long Zhang[c], Zhang-Zhen He[a], and Wen-Dan Cheng*[a]

[a]State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, P. R. China
[b]University of Chinese Academy of Sciences, Beijing, 100039, P. R. China.
[c]College of Electronics and Information Science, Fujian Jiangxia University, Fuzhou 350108, P.R. China.
E-mail: cwd@fjirsm.ac.cn

Supporting Information

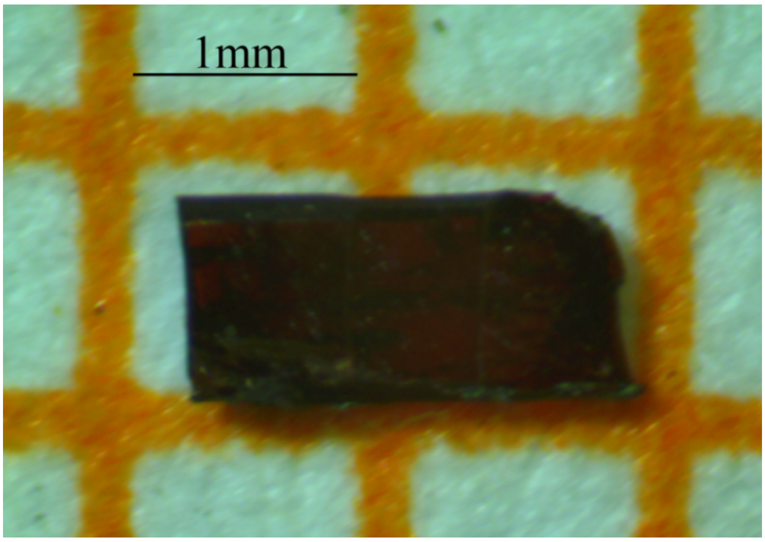

Fig. S1 Photograph of crystal for $Ba_5In_4Te_4S_7$.

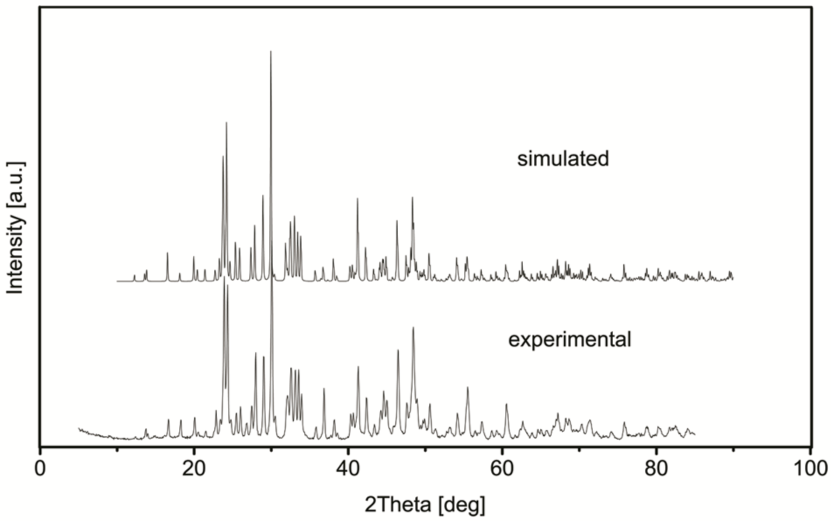

Fig. S2 Experimented (lower) and simulated (upper) X-ray (λ=1.5418 Å) diffraction patterns for $Ba_5In_4Te_4S_7$.

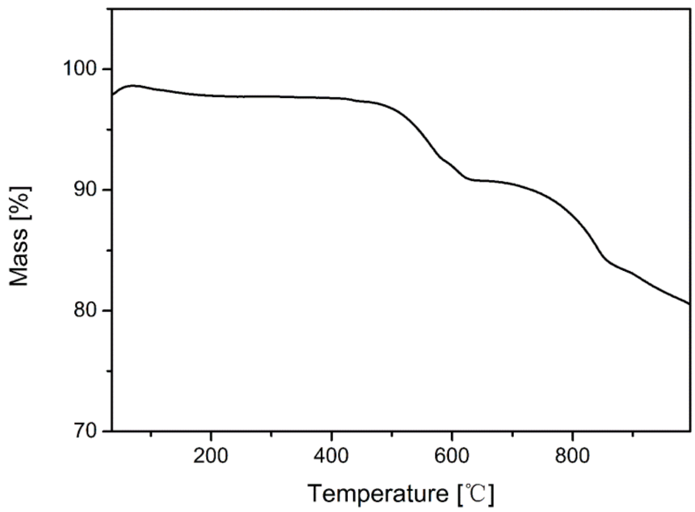

Fig. S3 TGA of $Ba_5In_4Te_4S_7$ in flowing N_2 atmosphere.

Table S1 Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for $Ba_5In_4Te_4S_7$

	x	y	z	U(eq)
Ba(1)	1	1	0.8420(1)	0.023(1)
Ba(2)	0.8149(1)	1	0.4940(1)	0.015(1)
Ba(3)	0.8859(1)	1	0.9941(1)	0.014(1)
In(1)	0.9457(1)	0.5000	0.3558(1)	0.014(1)
In(2)	0.8017(1)	0.5000	0.9749(1)	0.014(1)
Te(1)	0.9109(1)	1	0.4974(1)	0.016(1)
Te(2)	0.7595(1)	1	0.9157(1)	0.020(1)
S(1)	1	0.5000	0.5256(4)	0.019(1)
S(2)	0.9477(1)	0.5000	0.0161(2)	0.004(1)
S(3)	0.8486(1)	0.5000	0.7415(3)	0.014(1)
S(4)	0.8414(1)	0.5000	1.2277(3)	0.015(1)

Table S2 Selected bond lengths [Å] and angles (deg) for $Ba_5In_4Te_4S_7$.

Ba(1)-S(1)	3.192(2)	S(1)-Ba(1)-S(1)#1	86.54(8)
Ba(1)-S(2)#2	3.2557(13)	S(1)-Ba(1)-S(2)#2	79.94(4)
Ba(2)-Te(1)	3.7559(7)	S(3)-Ba(2)-Te(1)	66.30(4)
Ba(2)-Te(2)	3.7801(9)	Te(1)-Ba(2)-Te(2)	124.59(2)
In(1)-S(1)	2.4631(17)	S(1)-In(1)-S(2)	118.58(8)
In(1)-S(2)	2.496(2)	S(1)-In(1)-Te(1)	103.46(4)
In(1)-Te(1)	2.7791(5)	S(2)-In(1)-Te(1)	112.95(3)
In(2)-Te(2)	2.7759(5)	S(3)-In(2)-Te(2)	108.37(4)
Ba(3)-In(2)	3.9566(6)	S(3)-Ba(3)-In(2)	38.17(4)
Ba(1)-Ba(3)	4.5999(6)	S(1)-Ba(1)-Ba(3)	100.183(11)

Symmetry transformations used to generate equivalent atoms:

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