Electronic Supporting information

$BaLiTe_2O_5X$ (X = Cl, Br): Mixed alkali/alkaline-earth metal tellurite halides with $[Te_2O_5]_\infty$ chains

Ting Wang,[a] *Yi-Gang Chen,*[*a] *Yao Guo,*[b] *Fang Wang,*[b] *Qi Song,*[a] *Ying-Jie Jia,*[a] *and Xian-Ming Zhang*[*a]

[a]Key Laboratory of Magnetic Molecules and Magnetic Information Material of Ministry of Education, School of Chemistry and Material Science, Shanxi Normal University, Linfen 041004, China

[b]School of Chemical and Environmental Engineering, Anyang Institute of Technology, Anyang 455000, China

Table S1. Selected bond distances (Å) and important Angles (deg) for $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

Table S2. Energy-Dispersive Spectrometry (EDS) data for $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

Fig. S1. The images for $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

Fig. S2. Energy-Dispersive Spectrometry (EDS) plot of $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

Fig. S3. Experimental and simulated PXRD patterns of $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

Fig. S4. Structure of Li_2TeO_3.

Fig. S5. Structure of $Li_3(TeO_3)(OH)$.

Fig. S6. Structure of $Li_2Te_2O_5$.

Fig. S7. Structure of $Li_7(TeO_3)_3F$.

Fig. S8. TGA and DSC curves of $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

Fig. S9. IR spectra of $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

Table S1. Selected bond distances (Å) and important Angles (deg) for $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

$BaLiTe_2O_5Cl$

Te(1)−O(1)	1.891(2)	Ba(1)−O(2)	2.797(2)
Te(1)−O(2)	1.879(2)	Ba(1)−O(3)	3.048(2)
Te(1)−O(3)	1.833(2)	Ba(1)−O(4)	2.709(2)
Te(2)−O(5)	1.850(2)	Ba(1)−O(5)	2.707(2)
Te(2)−O(1c)	2.124(2)	Ba(1)−O(1a)	2.816(2)
Te(2)−O(1e)	2.124(2)	Ba(1)−O(1c)	3.219(2)
Te(2)−O(2b)	2.136(2)	Ba(1)−O(1d)	2.816(2)
Te(2)−O(4a)	1.856(2)	Ba(1)−O(1e)	3.219(2)
Te(2)−O(4d)	1.856(2)	Ba(1)−O(3a)	2.962(2)
Li(1)−O(3)	1.853(6)	Ba(1)−O(3d)	2.962(2)
Li(1)−O(4c)	2.007(6)	Ba(1)−O(4c)	2.973(2)
Li(1)−O(4e)	2.007(6)	Ba(1)−O(4e)	2.973(2)
Li(1)−O(5c)	2.002(6)	Ba(1)−O(5b)	2.969(2)
Li(1)−O(5e)	2.002(6)	Ba(1)−Cl(1)	3.622(9)
Li(1)−Cl(1f)	2.539(6)		
O(2)−Te(1)−O(1)	94.19(10)	O(5)−Te(2)−O(2b)	81.05(9)
O(3)−Te(1)−O(2)	94.36(10)	O(5)−Te(2)−O(4d)	108.67(10)
O(3)−Te(1)−O(1)	92.09(10)	O(3)−Li(1)−O(4c)	107.6(3)
O(1c)−Te(2)−O(2b)	160.48(9)	O(3)−Li(1)−O(5c)	103.9(3)

O(4d)−Te(2)−O(1c)	84.34(9)	O(5c)−Li(1)−O(4c)	107.5(3)
O(4d)−Te(2)−O(2b)	88.23(9)	O(3)−Li(1)−Cl(1f)	125.4(3)
O(5)−Te(2)−O(1c)	84.27(9)	O(5c)−Li(1)−Cl(1f)	104.7(2)

Symmetry codes: a) −1/2+x, 1/2−y, −1/2+z; b) 2–x, −y, 2−z; c) 3/2−x, 1/2+y, 3/2-z; d) 1/2+x, 1/2−y, 1/2 +z; e) 3/2−x, −1/2+y, 3/2−z; f) 2−x, 1−y, 1–z.

$BaLiTe_2O_5Br$

Te(1)−O(1)	1.828(4)	Li(1)−Br(1a)	2.728(10)
Te(1)−O(2)	1.889(4)	Ba(1)−O(3)	3.208(4)
Te(1)−O(3)	1.901(4)	Ba(1)−O(4)	2.713(4)
Te(2)−O(2)	1.862(4)	Ba(1)−O(1a)	2.949(4)
Te(2)−O(3)	2.124(4)	Ba(1)−O(1b)	3.058(4)
Te(2)−O(4)	1.847(4)	Ba(1)−O(1e)	3.058(4)
Te(2)−O(2c)	2.132(4)	Ba(1)−O(2b)	2.819(4)
Te(2)−O(2g)	2.132(4)	Ba(1)−O(2e)	2.819(4)
Li(1)−O(1)	1.848(10)	Ba(1)−O(3a)	2.832(4)
Li(1)−O(2k)	2.010(10)	Ba(1)−O(4d)	3.003(4)
Li(1)−O(4f)	1.982(10)	Ba(1)−O(5a)	2.963(4)
Li(1)−O(4j)	1.982(10)	Ba(1)−O(5c)	2.711(4)
Li(1)−O(5h)	2.010(10)	Ba(1)−O(5g)	2.711(4)
Li(1)−Br(1i)	2.728(11)	Ba(1)−Br(1a)	3.7099(7)
O(1)−Te(1)−O(2)	94.04(18)	O(5)−Te(2)−O(2g)	87.78(16)
O(1)−Te(1)−O(3)	92.11(17)	O(5)−Te(2)−O(3)	83.94(15)

O(2)−Te(1)−O(3)	93.71(18)	O(1)−Li(1)−O(4j)	105.1(5)
O(3)−Te(2)−O(2g)	159.64(16)	O(1)−Li(1)−O(5k)	108.6(5)
O(4)−Te(2)−O(2g)	81.25(16)	O(4j)−Li(1)−O(5k)	108.9(5)
O(4)−Te(2)−O(3)	83.79(16)	O(1)−Li(1)−Br(1l)	123.9(5)
O(4)−Te(2)−O(5)	108.52(17)		

Symmetry codes: a) 1−x, 1−y, 1–z; b) 1/2−x, 1/2+y, 1/2–z; c) −1/2+x, 1/2−y, −1/2+z; d) 1−x, −y, 1–z; e) 1/2−x, −1/2+y, 1/2–z; f) +x, −1+y, +z; g) 1/2+x, 1/2−y, 1/2+z; h) 1/2+x, 3/2−y, 1/2+z; i) 1/2−x, −1/2+y, 3/2–z; j) +x, 1+y, +z; k) −1/2+x, 3/2−y, −1/2+z; l) 1/2−x, 1/2+y, 3/2–z.

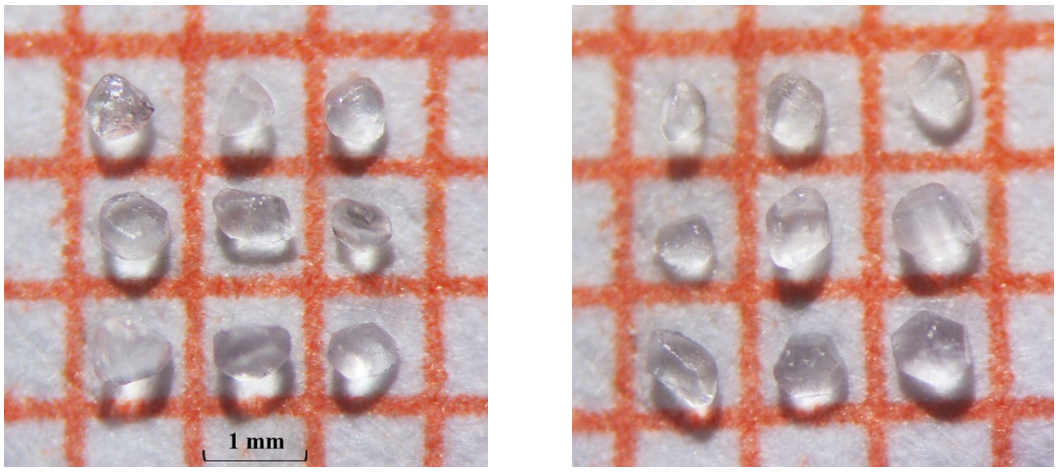
Table S2. Energy-Dispersive Spectrometry (EDS) data for $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

$BaLiTe_2O_5Cl$

Point 1				Point 2			
Element	Weight	Atomic	Formula	Element	Weight	Atomic	Formul
Ba L	27.81	11.72	1.0	Ba L	28.05	11.85	1.01
Te L	50.09	22.73	1.94	Te L	50.39	22.80	1.94
Cl K	7.26	11.85	1.01	Cl K	6.96	11.78	1.0
O K	14.84	53.70		O K	14.6	53.57	
Totals	100			Totals	100		
Point 3							
Element	Weight	Atomic	Formula				
Ba L	27.84	11.74	1.0				
Te L	50.19	22.76	1.94	Average ratio:			
Cl K	7.16	11.82	1.01	$Ba_{1.0}Te_{1.94}Cl_{1.0}$			
O K	14.81	53.68					
Totals	100						

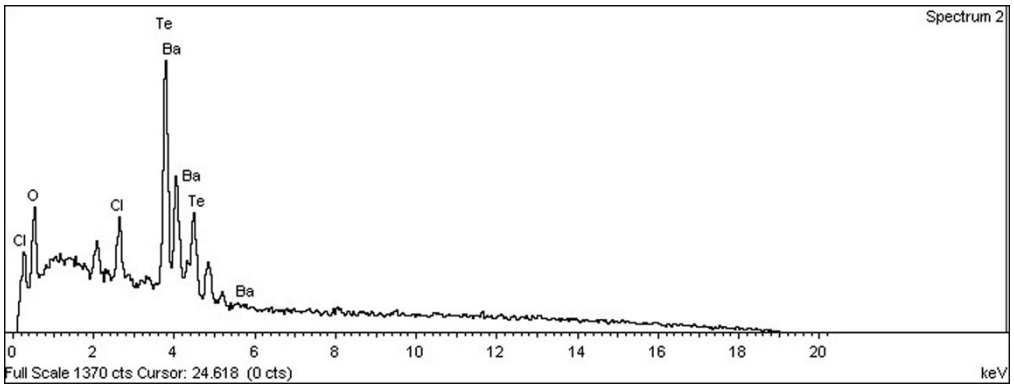
$BaLiTe_2O_5Br$

Point 1				Point 2			
Element	Weight	Atomic	Formula	Element	Weight	Atomic	Formula
Ba L	23.98	10.33	1.0	Ba L	25.13	11.05	1.01
Te L	45.83	21.26	2.06	Te L	45.48	21.53	1.98
Br L	14.63	10.83	1.05	Br L	28.05	10.90	1.0
O K	15.56	57.57		O K	14.97	56.52	
Totals	100			Totals	100		
Point 3							
Element	Weight	Atomic	Formula				
Ba L	25.31	11.40	1.0				
Te L	45.49	22.07	1.94	Average ratio:			
Br L	15.00	11.62	1.02	$Ba_{1.0}Te_{1.99}Br_{1.02}$			
O K	14.20	54.91					
Totals	100						

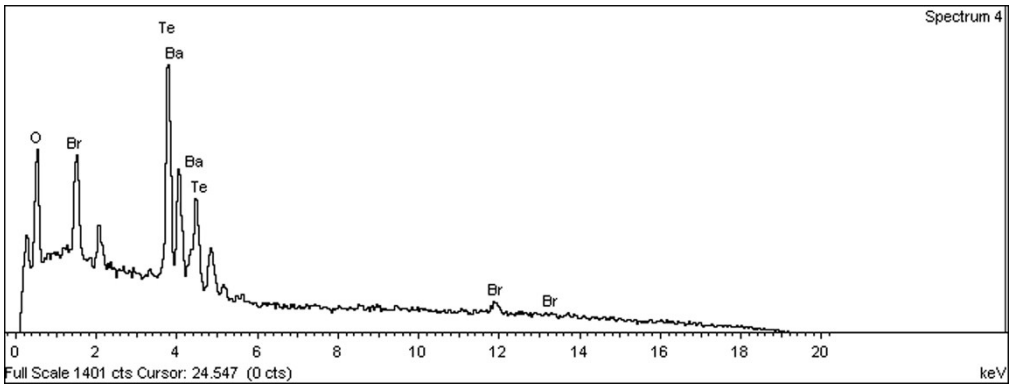


$BaLiTe_2O_5Cl$ $BaLiTe_2O_5Br$

Fig. S1. The images for $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.



$BaLiTe_2O_5Cl$



BaLiTe2O5Br

Fig. S2. Energy-Dispersive Spectrometry (EDS) plot of $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

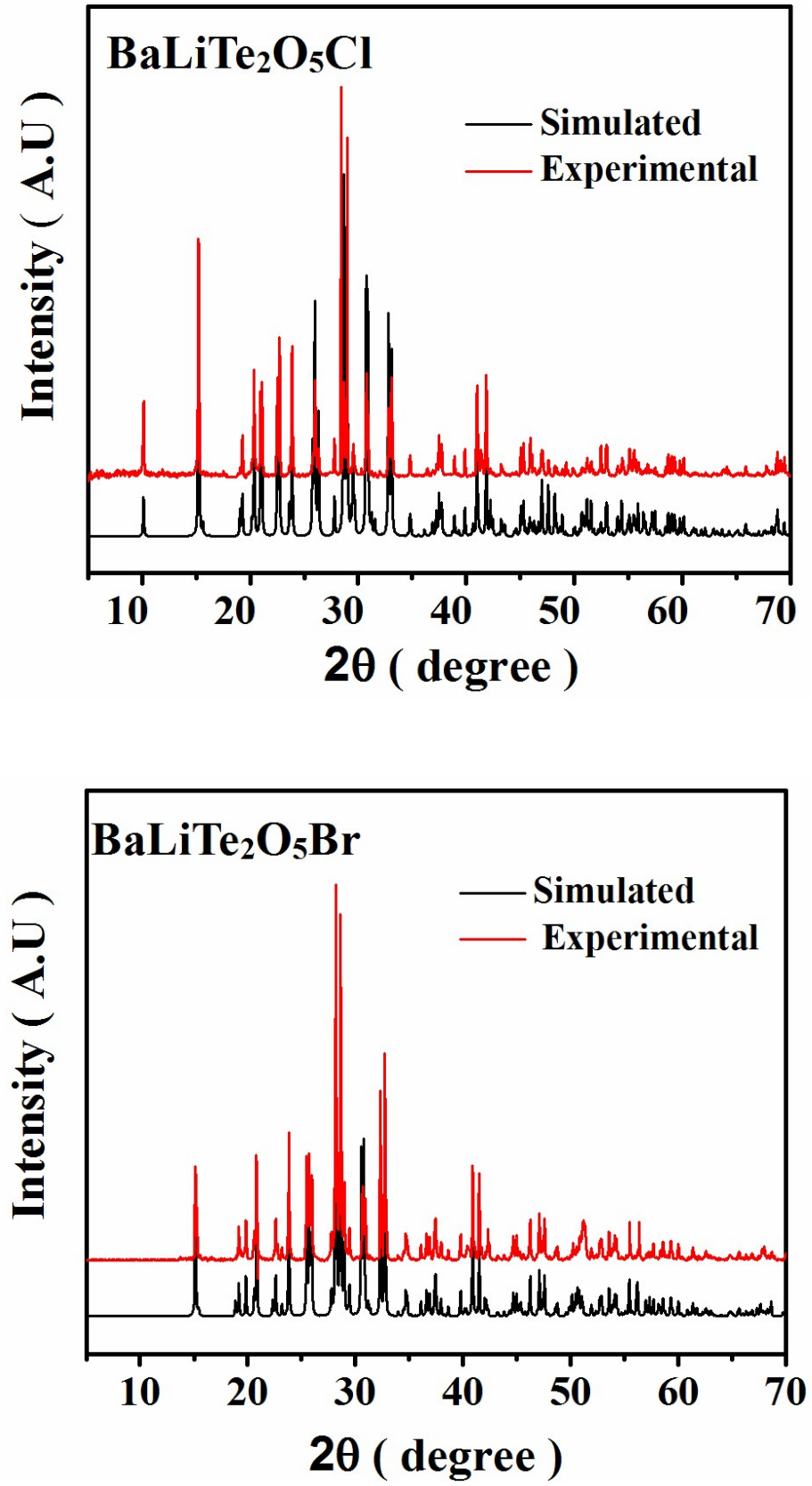
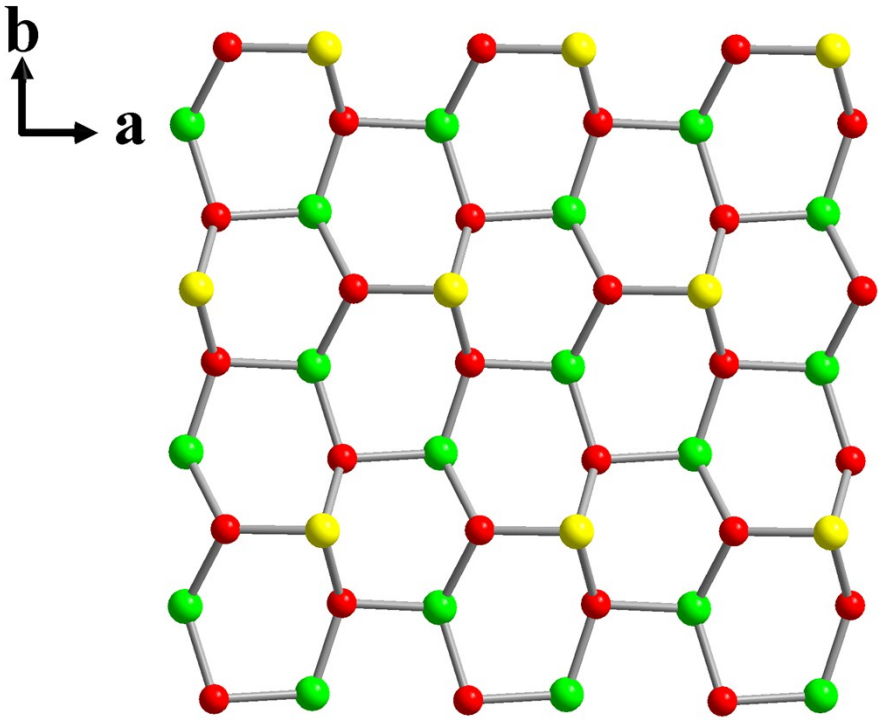
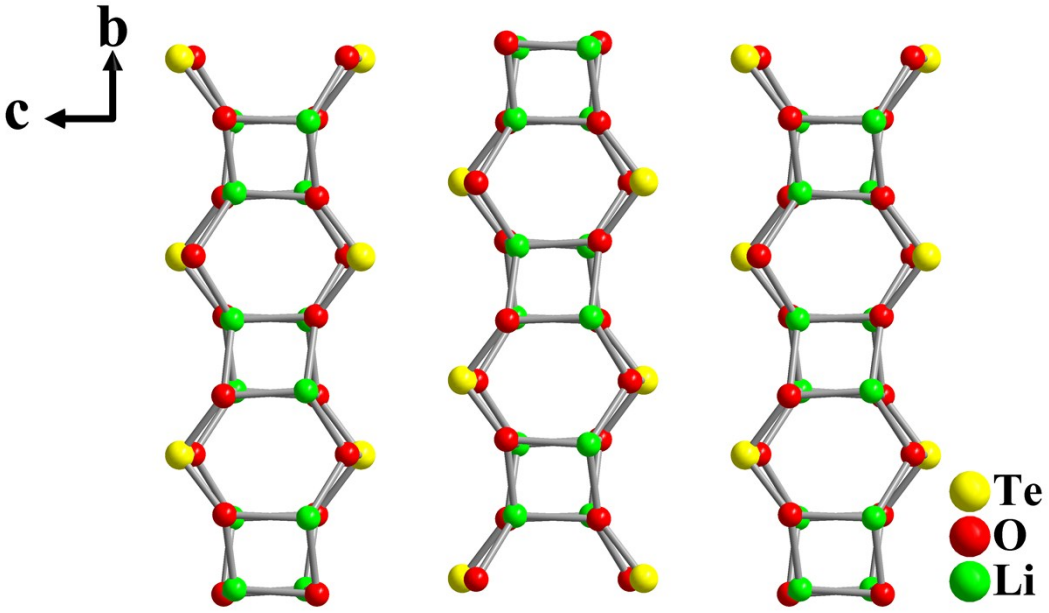


Fig. S3. Experimental and simulated PXRD patterns of $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

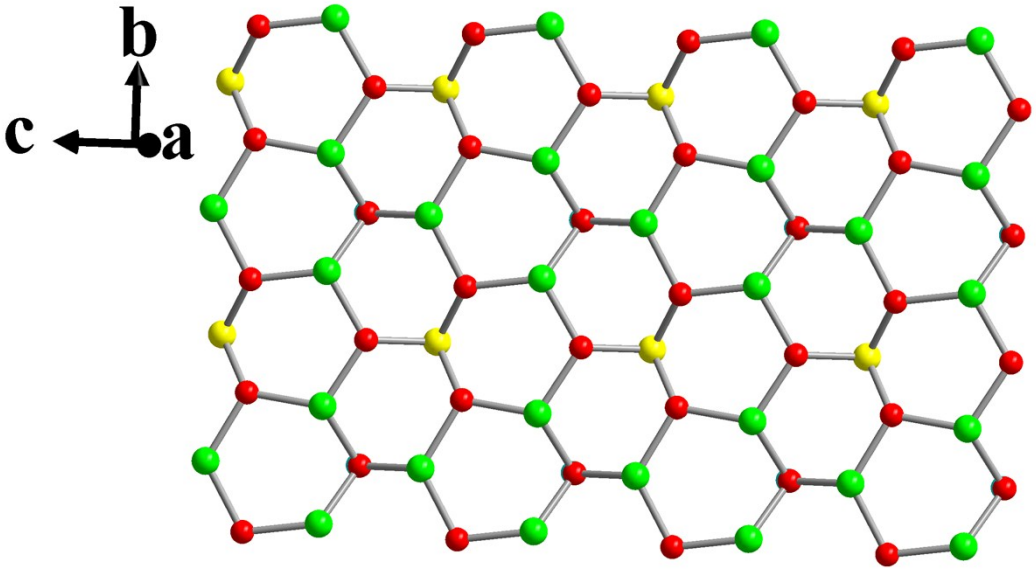


(a) Monolayer in Li_2TeO_3

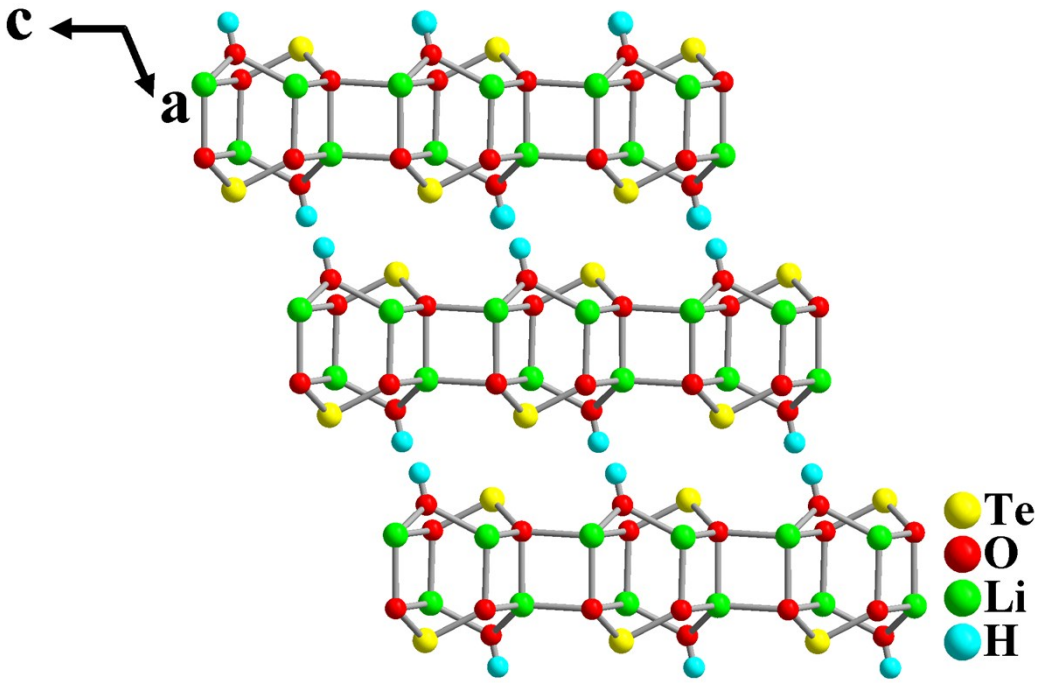


(b) 2D double layer in Li_2TeO_3

Fig. S4. Structure of Li_2TeO_3.

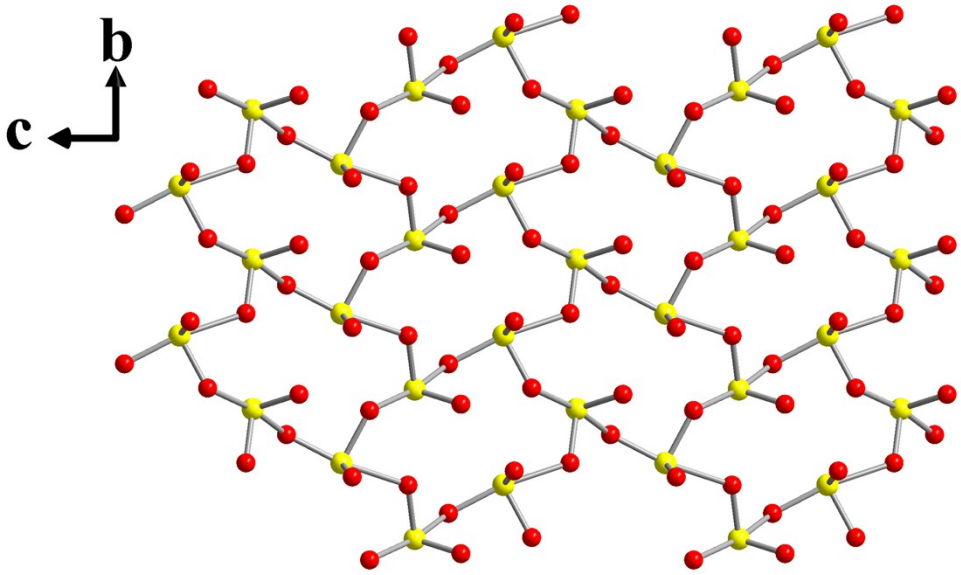


(a) Monolayer in $Li_3(TeO_3)(OH)$

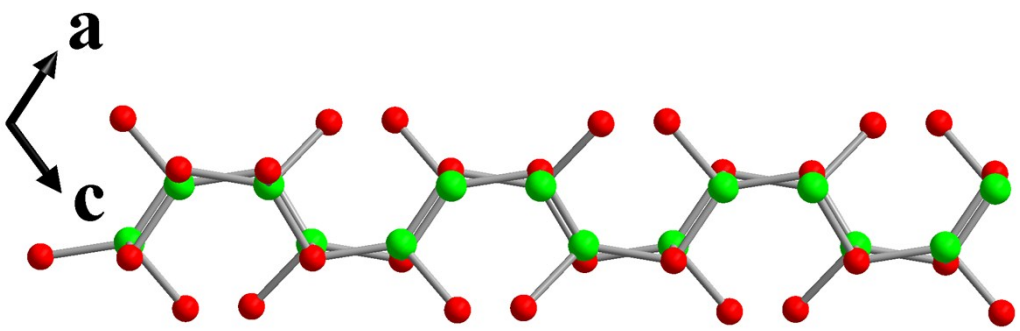


(b) 2D double layer in $Li_3(TeO_3)(OH)$

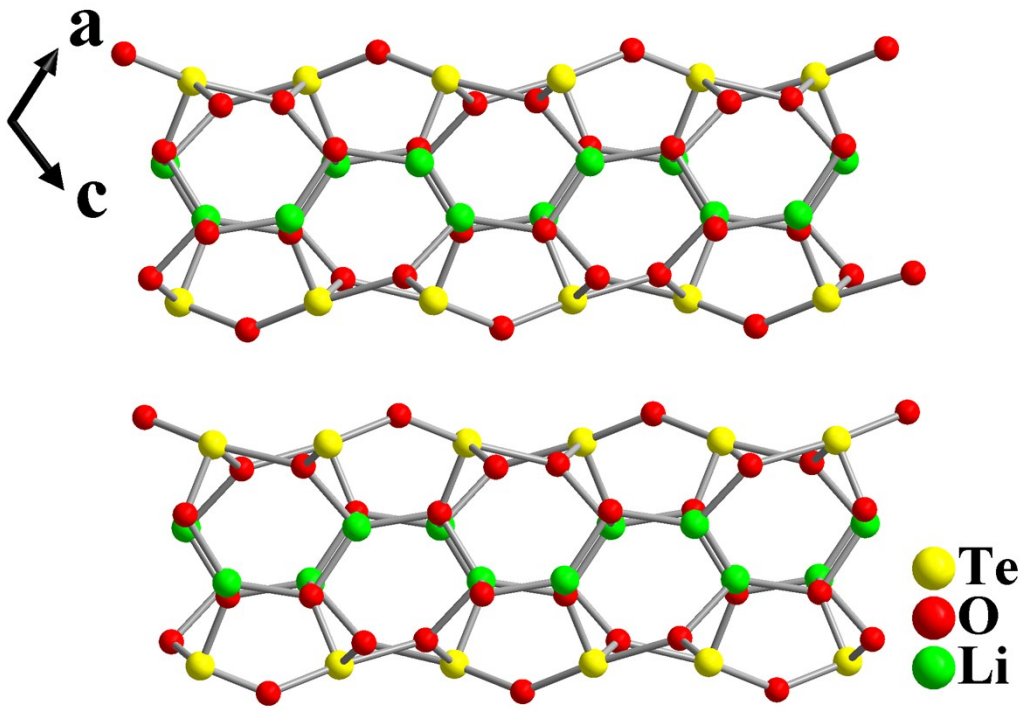
Fig. S5. Structure of $Li_3(TeO_3)(OH)$.



(a) Te−O layer in $Li_2Te_2O_5$



(b) Li−O layer in $Li_2Te_2O_5$



(c) 2D double layer in $Li_2Te_2O_5$

Fig. S6. Structure of $Li_2Te_2O_5$.

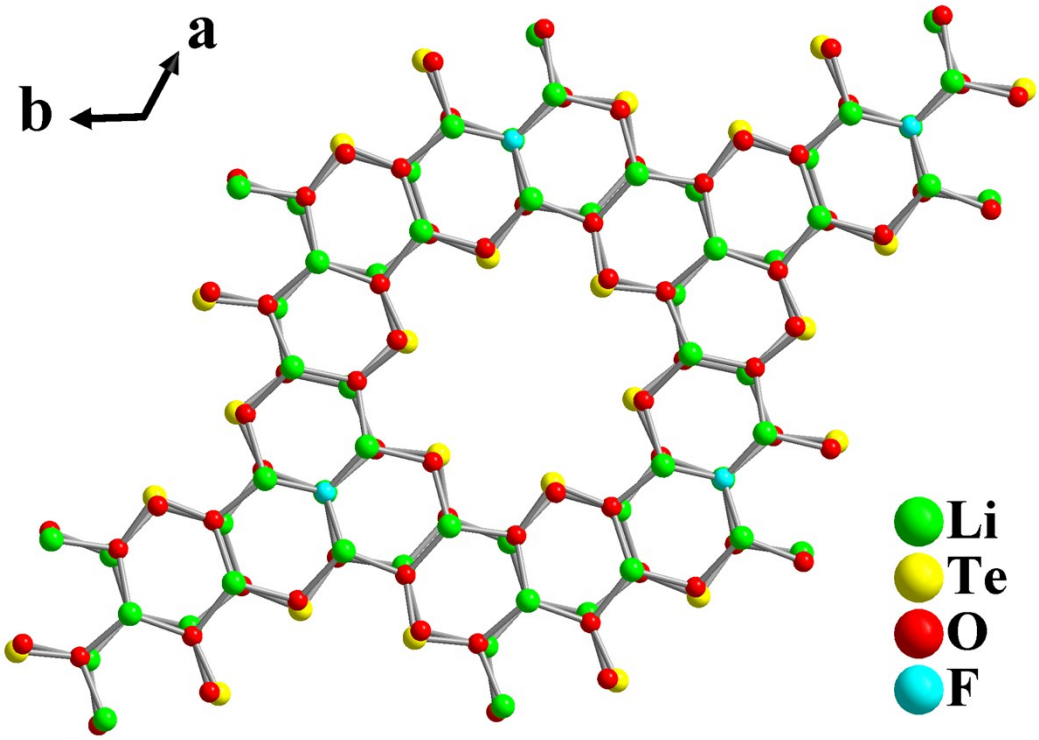


Fig. S7. 3D Structure of $Li_7(TeO_3)_3F$.

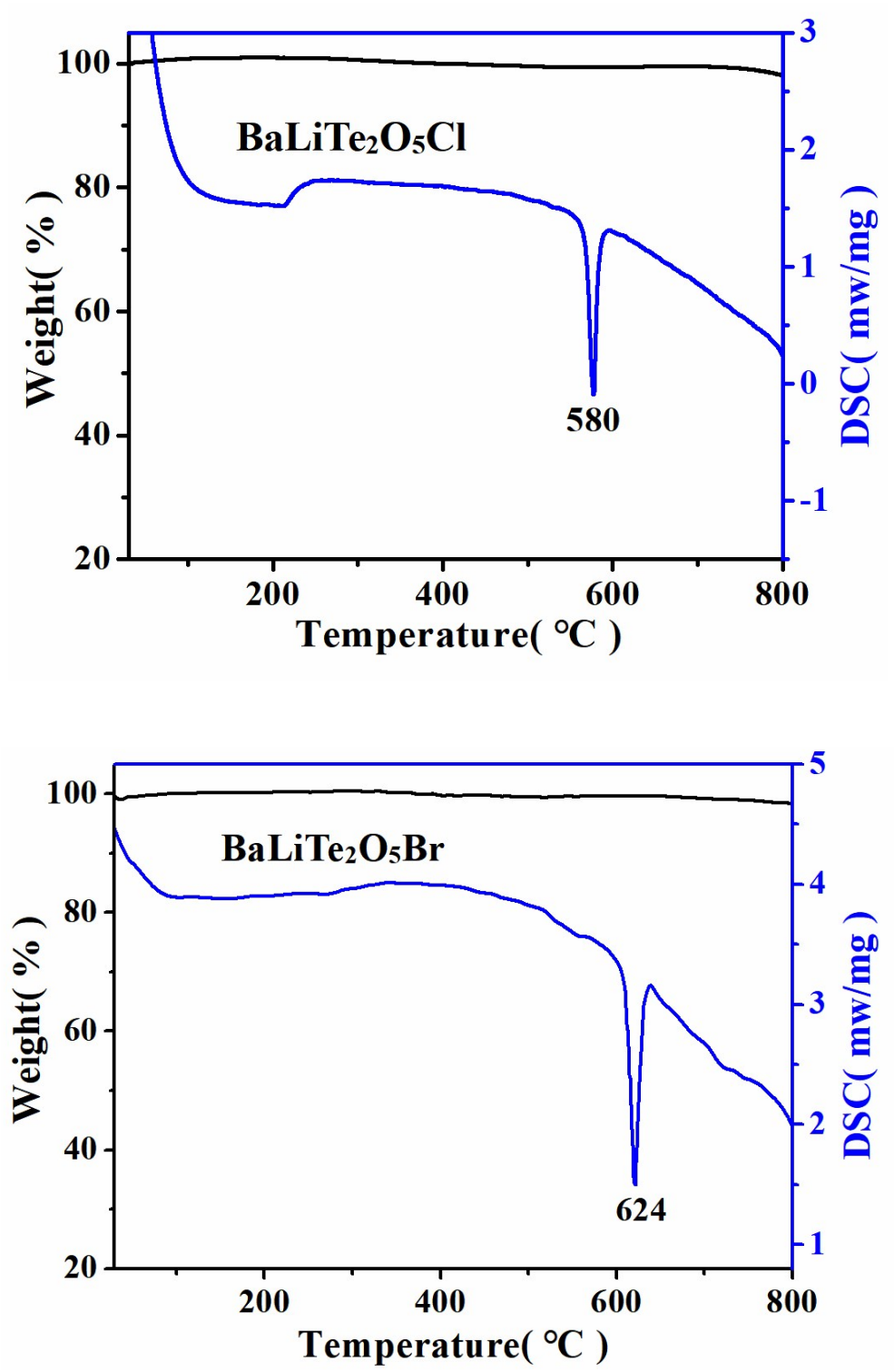


Fig. S8. TGA and DSC curves of $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.

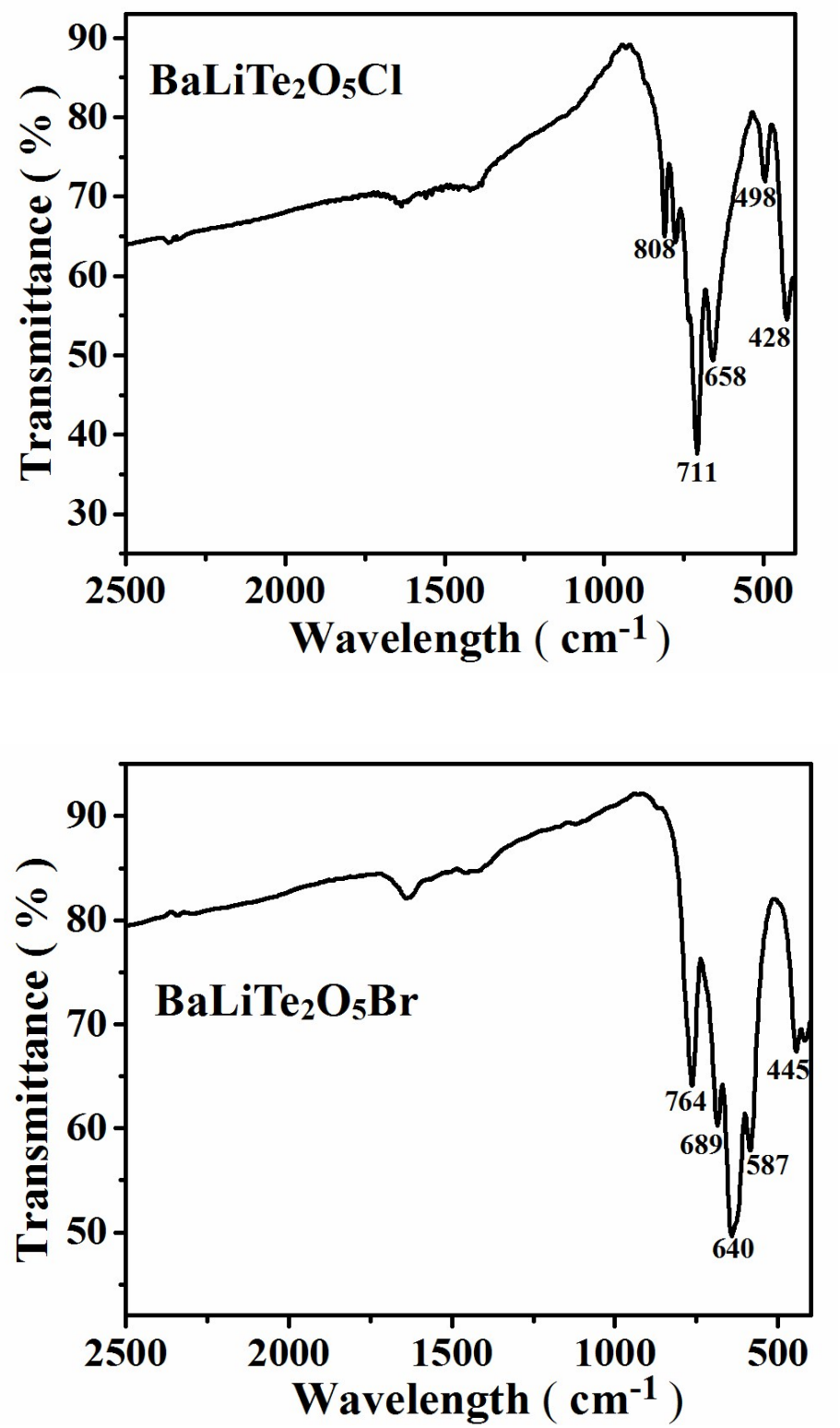


Fig. S9. IR spectra of $BaLiTe_2O_5Cl$ and $BaLiTe_2O_5Br$.