Supporting Information for:

Structural Analysis, Characterization and First-Principles Calculation on Bismuth Tellurium Oxides, $Bi_6Te_2O_{15}$

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $Bi_6Te_2O_{15}$.

atom	x	y	z	$U_{(eq)}$
Bi(1)	0.3798(1)	0.5061(1)	0.7172(1)	0.01985(1)
Bi(2)	0.6384(1)	0.7500	0.2767(1)	0.02068(1)
Bi(3)	0.3899(1)	0.7500	0.7316(1)	0.01973(1)
Bi(4)	0.6161(1)	0.3777(1)	0.7659(1)	0.02154(1)
Te(1)	0.6319(1)	0.6280(1)	0.7514(2)	0.01999(1)
O(1)	0.5777(9)	0.6801(4)	1.0138(17)	0.02498(2)
O(2)	0.6901(8)	0.5781(4)	0.4910(15)	0.01923(2)
O(3)	0.5023(9)	0.6624(4)	0.5422(15)	0.02428(2)
O(4)	0.7597(8)	0.5934(4)	0.9553(16)	0.01830(2)
O(5)	0.5105(9)	0.5734(4)	0.8916(17)	0.03174(2)
O(6)	0.7467(8)	0.6878(4)	0.6174(16)	0.02544(2)
O(7)	0.5649(8)	0.4648(4)	0.6506(17)	0.01591(2)
O(8)	0.8253(11)	0.7500	0.1470(20)	0.01687(3)

$U_{(eq)}$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S2. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Bi_6Te_2O_{15}$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Bi(1)	20(1)	17(1)	18(1)	0(1)	1(1)	-1(1)
Bi(2)	21(1)	16(1)	18(1)	0	0(1)	0
Bi(3)	20(1)	17(1)	18(1)	0	0(1)	0
Bi(4)	22(1)	16(1)	18(1)	0(1)	0(1)	0(1)
Te(1)	20(1)	14(1)	17(1)	1(1)	0(1)	0(1)
O(1)	25(5)	19(5)	21(5)	-4(4)	3(4)	-2(4)
O(2)	19(4)	27(5)	11(4)	-6(4)	-2(3)	-1(4)
O(3)	24(5)	27(5)	11(4)	0(4)	-2(4)	0(4)
O(4)	18(4)	21(5)	20(5)	4(4)	-3(4)	5(4)
O(5)	32(5)	17(5)	22(5)	-1(4)	0(4)	-10(4)
O(6)	25(5)	20(4)	13(4)	-1(4)	-2(4)	-4(4)
O(7)	16(4)	26(5)	22(5)	-2(4)	1(4)	-2(4)
O(8)	17(6)	24(7)	16(6)	0	1(5)	0

Table S3. Local dipole moment calculation

The local dipole moment of the square pyramidal of $[Bi(1)O_5]^{7-}$ without lone-pair electron or with lone-pair electron is calculated.

$Bi(1)O_5$ in $Bi_6Te_2O_{15}$ without lone pair			Cart. Coord.			Distance	Unit vector				Dipole moment between two atoms		
Z	atom	charges	x	y	z	Å	x	y	z	Unitized Vector	C_grav	C_charge	u_debye
83	Bi(1)	3.029	4.019	-0.138	3.862								
8	O2	-0.521	3.280	1.772	2.741	2.335	-0.317	0.818	-0.480	1.000	0.088	0.096	8.309
8	O4	-0.308	2.749	-2.119	2.933	2.530	-0.502	-0.783	-0.367	1.000	0.088	0.094	6.645
8	O5	-0.630	5.403	-1.666	4.800	2.265	0.611	-0.675	0.414	1.000	0.088	0.097	9.142
8	O7A	-0.819	4.605	-0.798	1.881	2.169	0.270	-0.305	-0.913	1.000	0.088	0.099	10.547
8	O7B	-0.751	5.978	0.798	3.503	2.200	0.890	0.425	-0.163	1.000	0.088	0.099	10.046
				Cell Volume		1293.613			Dipole Moment			Magnitude	
				Z		4.000			x	y	z		
				Total Dipole Moments =Polarization(P) =		0.057	Debye/A^3		11.406	-3.510	-13.914	**18.331**	Debye

$Bi(1)O_5$(Lp) in $Bi_6Te_2O_{15}$ with lone pair			Cart. Coord.			Distance	Unit vector				Dipole moment between two atoms		
Z	atom	charges	x	y	z	Å	x	y	z	Unitized Vector	C_grav	C_charge	u_debye
83	Bi(1)	3.029	0.000	0.000	0.000								
8	O2	-0.521	0.740	-1.909	1.121	2.335	0.317	-0.818	0.480	1.000	0.088	0.096	8.309
8	O4	-0.308	1.271	1.981	0.929	2.530	0.502	0.783	0.367	1.000	0.088	0.094	6.645
8	O5	-0.630	-1.384	1.528	-0.938	2.265	-0.611	0.675	-0.414	1.000	0.088	0.097	9.142
8	O7A	-0.819	-0.586	0.660	1.981	2.169	-0.270	0.305	0.913	1.000	0.088	0.099	10.547
8	O7B	-0.751	-1.958	-0.936	0.359	2.200	-0.890	-0.425	0.163	1.000	0.088	0.099	10.046
2	LP	-2.000	0.451	-0.311	-0.812	0.980	0.460	-0.318	-0.829	1.000	0.024	0.048	9.524
			-4.248										
				Cell Volume		1293.613			Dipole Moment			Magnitude	
				Z		4.000			x	y	z		
				Total Dipole Moments =Polarization(P) =		0.029	Debye/A^3		-7.020	0.484	6.021	**9.261**	Debye

The local dipole moment of the square pyramidal of $[Bi(2)O_5]^{7-}$ without lone-pair electron or with lone-pair electron is calculated.

$Bi(2)O_5$ in $Bi_6Te_2O_{15}$ without lone pair			Cart. Coord.			Distance	Unit vector				Dipole moment between two atoms		
Z	atom	charges	x	y	z	Å	x	y	z	Unitized Vector	C_grav	C_charge	u_debye
83	Bi(2)	2.942	3.82678	5.6735	-6.8742								
8	O1A	-0.709	4.46908	4.08735	-5.45836	2.221	0.289	-0.714	0.637	1.000	0.088	0.098	9.651
8	O1B	-0.709	4.46908	7.25965	-5.45836	2.221	0.289	0.714	0.637	1.000	0.088	0.098	9.651
8	O6A	-0.267	2.68091	4.2613	-8.70858	2.583	-0.444	-0.547	-0.710	1.000	0.088	0.094	6.226
8	O6B	-0.267	2.68091	7.0857	-8.70858	2.583	-0.444	0.547	-0.710	1.000	0.088	0.094	6.226
8	O8	-0.989	1.84904	5.6735	-6.17416	2.098	-0.943	0.000	0.334	1.000	0.088	0.101	11.689
				Cell Volume		1293.613			Dipole Moment			Magnitude	
				Z		4.000			x	y	z		
				Total Dipole Moments = Polarization(P) =		0.041	Debye/A^3		-10.960	0.000	7.362	**13.203**	Debye

$Bi(2)O_5$(Lp) in $Bi_6Te_2O_{15}$ with lone pair			Cart. Coord.			Distance	Unit vector				Dipole moment between two atoms		
Z	atom	charges	x	y	z	Å	x	y	z	Unitized Vector	C_grav	C_charge	u_debye
83	Bi(2)	2.942	0.000	0.000	0.000								
8	O1A	-0.709	-0.642	1.586	-1.416	2.221	-0.289	0.714	-0.637	1.000	0.088	0.098	9.651
8	O1B	-0.709	-0.642	-1.586	-1.416	2.221	-0.289	-0.714	-0.637	1.000	0.088	0.098	9.651
8	O6A	-0.267	1.146	1.412	1.834	2.583	0.444	0.547	0.710	1.000	0.088	0.094	6.226
8	O6B	-0.267	1.146	-1.412	1.834	2.583	0.444	-0.547	0.710	1.000	0.088	0.094	6.226
8	O8	-0.989	1.978	0.000	-0.700	2.098	0.943	0.000	-0.334	1.000	0.088	0.101	11.689
2	LP	-2.000	-0.979	0.000	-0.045	0.980	-0.999	0.000	-0.046	1.000	0.024	0.048	9.509
			-3.050										
				Cell Volume		1293.613			Dipole Moment			Magnitude	
				Z		4.000			x	y	z		
				Total Dipole Moments =Polarization(P) =		0.025	Debye/A^3		1.461	0.000	-7.798	**7.934**	Debye

The local dipole moment of the square pyramidal of $[Bi(3)O_5]^{7-}$ without lone-pair electron or with lone-pair electron is calculated.

$Bi(3)O_5$ in $Bi_6Te_2O_{15}$ without lone pair			Cart. Coord.			Distance	Unit vector				Dipole moment between two atoms		
Z	atom	charges	x	y	z	Å	x	y	z	Unitized Vector	C_grav	C_charge	u_debye
83	Bi(3)	2.878	1.165	5.674	-4.138								
8	O3A	-0.709	-0.024	7.662	-5.157	2.531	-0.470	0.786	-0.403	1.000	0.088	0.098	10.931
8	O3B	-0.709	-0.024	3.685	-5.157	2.531	-0.470	-0.786	-0.403	1.000	0.088	0.098	10.931
8	O6A	-0.267	2.681	4.261	-3.324	2.226	0.681	-0.634	0.365	1.000	0.088	0.094	5.305
8	O6B	-0.267	2.681	7.086	-3.324	2.226	0.681	0.634	0.365	1.000	0.088	0.094	5.305
8	O8	-0.989	1.849	5.674	-6.174	2.148	0.318	0.000	-0.948	1.000	0.088	0.101	11.912
				Cell Volume		1293.613			Dipole Moment			Magnitude	
				Z		4.000			x	y	z		
				Total Dipole Moments =Polarization(P) =		0.050	Debye/A^3		0.751	0.000	-16.223	**16.240**	Debye

$Bi(3)O_5$ in $Bi_6Te_2O_{15}$ with lone pair			Cart. Coord.			Distance	Unit vector				Dipole moment between two atoms		
Z	atom	charges	x	y	z	Å	x	y	z	Unitized Vector	C_grav	C_charge	u_debye
83	Bi(3)	2.878	0.000	0.000	0.000								
8	O3A	-0.709	1.189	-1.988	1.020	2.531	0.470	-0.786	0.403	1.000	0.088	0.098	10.931
8	O3B	-0.709	1.189	1.988	1.020	2.531	0.470	0.786	0.403	1.000	0.088	0.098	10.931
8	O6A	-0.267	-1.516	1.412	-0.813	2.226	-0.681	0.634	-0.365	1.000	0.088	0.094	5.305
8	O6B	-0.267	-1.516	-1.412	-0.813	2.226	-0.681	-0.634	-0.365	1.000	0.088	0.094	5.305
8	O8	-0.989	-0.684	0.000	2.037	2.148	-0.318	0.000	0.948	1.000	0.088	0.101	11.912
2	LP	-2.000	0.470	0.000	-0.860	0.980	0.479	0.000	-0.878	1.000	0.024	0.048	9.510
			-2.847										
				Cell Volume		1293.613			Dipole Moment			Magnitude	
				Z		4.000			x	y	z		
				Total Dipole Moments =Polarization(P) =		0.027	Debye/A^3		3.808	0.000	7.877	**8.750**	Debye

The local dipole moment of the square pyramidal of $[Bi(4)O_5]^{7-}$ without lone-pair electron or with lone-pair electron is calculated.

$Bi(4)O_5$ in $Bi_6Te_2O_{15}$ without lone pair			Cart. Coord.			Distance	Unit vector				Dipole moment between two atoms		
Z	atom	charges	x	y	z	Å	x	y	z	Unitized Vector	C_grav	C_charge	u_debye
83	Bi(4)	2.770	1.229	2.775	3.953								
8	O2	-0.709	3.280	1.772	2.741	2.585	0.793	-0.388	-0.469	1.000	0.088	0.098	11.045
8	O3	-0.709	-0.024	3.685	5.611	2.269	-0.552	0.401	0.731	1.000	0.088	0.098	9.695
8	O4	-0.267	2.543	2.119	5.625	2.226	0.590	-0.295	0.751	1.000	0.088	0.093	5.203
8	O5	-0.267	-0.112	1.666	2.108	2.536	-0.529	-0.437	-0.727	1.000	0.088	0.093	5.927
8	O7	-0.989	0.686	0.798	4.573	2.142	-0.253	-0.923	0.290	1.000	0.088	0.101	11.776
				Cell Volume		1293.613			Dipole Moment			Magnitude	
				Z		4.000			x	y	z		
				pole Moments=Polarizati		0.050	Debye/A^3		0.364	-15.394	4.918	**16.165**	Debye

$Bi(4)O_5$ in $Bi_6Te_2O_{15}$ with lone pair			Cart. Coord.			Distance	Unit vector				Dipole moment between two atoms		
Z	atom	charges	x	y	z	Å	x	y	z	Unitized Vector	C_grav	C_charge	u_debye
83	Bi(4)	2.770	0.000	0.000	0.000								
8	O2	-0.709	-2.051	1.003	1.212	2.585	-0.793	0.388	0.469	1.000	0.088	0.098	11.045
8	O3	-0.709	1.253	-0.910	-1.659	2.269	0.552	-0.401	-0.731	1.000	0.088	0.098	9.695
8	O4	-0.267	-1.314	0.656	-1.672	2.226	-0.590	0.295	-0.751	1.000	0.088	0.093	5.203
8	O5	-0.267	1.340	1.109	1.845	2.536	0.529	0.437	0.727	1.000	0.088	0.093	5.927
8	O7	-0.989	0.543	1.977	-0.621	2.142	0.253	0.923	-0.290	1.000	0.088	0.101	11.776
2	LP	-2.000	0.057	-0.953	0.222	0.980	0.058	-0.972	0.227	1.000	0.024	0.047	9.495
			-4.025										
				Cell Volume		1293.613			Dipole Moment			Magnitude	
				Z		4.000			x	y	z		
				Total Dipole Moments =Polarization(P) =		0.021	Debye/A^3		0.187	6.163	-2.764	**6.757**	Debye

The local dipole moment of the octahedral of $[Te(1)O_6]^{6-}$ is also calculated.

$Te(1)O_6$ in $Bi_6Te_2O_{15}$			Cart. Coord.			Distance	Unit vector				Dipole moment between two ato		
Z	atom	charges	x	y	z	Å	x	y	z	Unitized Vector	C_grav	C_charge	u_debye
52	Te	5.797	-1.395	2.906	-4.031								
8	O1	-0.968	-0.822	4.087	-2.618	1.929	0.297	0.613	0.732	1.000	0.133	0.163	14.922
8	O2	-1.030	-2.012	1.772	-5.433	1.906	-0.323	-0.595	-0.736	1.000	0.133	0.163	15.236
8	O3	-0.945	-0.024	3.685	-5.157	1.938	0.708	0.402	-0.581	1.000	0.133	0.162	14.811
8	O4	-1.014	-2.749	2.119	-2.933	1.912	-0.708	-0.412	0.574	1.000	0.133	0.163	15.159
8	O5	-0.945	-0.112	1.666	-3.276	1.938	0.662	-0.640	0.389	1.000	0.133	0.162	14.806
8	O6	-0.895	-2.611	4.261	-4.752	1.958	-0.621	0.692	-0.368	1.000	0.133	0.161	14.558
				Cell Volume		1293.613			Dipole Moment			Magnitude	
				Z		4.000			x	y	z		
				Total Dipole Moments =Polarization(P) =		0.001	Debye/A^3		0.030	0.392	0.219	**0.450**	Debye

Table S4. Table of the calculation for BSI (Bond Stability Index) and GII (Global Instability Index)

BSI = 0.172		Bi(1)		Bi(2)	Bi(3)	Bi(4)		Te(1)					
GII = 0.279		1	1	1	1	1	1	1	1	$\sum_i(S_{ij}-s_{ij})^2$	$V_i=\sum_i S_{ij}$	$z_i=\sum_i s_{ij}$	V_i-z_i	$(V_i-z_i)^2$
O(1)	Total Connectivity			2				1	1					
	Each Connection			2				1	1					
	R_{ij}			2.221				1.929	1.929					
	S_{ij}			0.709				0.968	0.968		3.355			
	s_{ij}			0.656				1.345	1.345			4.000		
	$S_{ij}-s_{ij}$			0.054				-0.376	-0.376					
	$(S_{ij}-s_{ij})^2$			0.003				0.142	0.142	0.289			-0.645	0.416
2														
O(2)	Total Connectivity	1	1			1	1	1	1					
	Each Connection	1	1			1	1	1	1					
	R_{ij}	2.335	2.335			2.585	2.585	1.906	1.906					
	S_{ij}	0.521	0.521			0.265	0.265	1.030	1.030		3.634			
	s_{ij}	0.557	0.557			0.565	0.565	0.878	0.878			4.000		
	$S_{ij}-s_{ij}$	-0.036	-0.036			-0.299	-0.299	0.152	0.152				-0.366	0.134
	$(S_{ij}-s_{ij})^2$	0.001	0.001			0.090	0.090	0.023	0.023	0.228				
2														
O(3)	Total Connectivity				2	1	1	1	1					
	Each Connection				2	1	1	1	1					
	R_{ij}				2.531	2.269	2.269	1.938	1.938					
	S_{ij}				0.307	0.623	0.623	0.945	0.945		3.750			
	s_{ij}				0.418	0.634	0.634	0.948	0.948			4.000		
	$S_{ij}-s_{ij}$				-0.111	-0.011	-0.011	-0.003	-0.003				-0.250	0.063
	$(S_{ij}-s_{ij})^2$				0.012	0.000	0.000	0.000	0.000	0.025				
2														
O(4)	Total Connectivity	1	1			1	1	1	1					
	Each Connection	1	1			1	1	1	1					
	R_{ij}	2.530	2.530			2.226	2.226	1.912	1.912					
	S_{ij}	0.308	0.308			0.700	0.700	1.014	1.014		4.043			
	s_{ij}	0.557	0.557			0.565	0.565	0.878	0.878			4.000		
	$S_{ij}-s_{ij}$	-0.249	-0.249			0.135	0.135	0.136	0.136				0.043	0.002
	$(S_{ij}-s_{ij})^2$	0.062	0.062			0.018	0.018	0.018	0.018	0.198				
2														
O(5)	Total Connectivity	1	1			1	1	1	1					
	Each Connection	1	1			1	1	1	1					
	R_{ij}	2.265	2.265			2.536	2.536	1.938	1.938					
	S_{ij}	0.630	0.630			0.303	0.303	0.945	0.945		3.755			
	s_{ij}	0.557	0.557			0.565	0.565	0.878	0.878			4.000		
	$S_{ij}-s_{ij}$	0.073	0.073			-0.262	-0.262	0.067	0.067				-0.245	0.060
	$(S_{ij}-s_{ij})^2$	0.005	0.005			0.069	0.069	0.004	0.004	0.157				
2														
O(6)	Total Connectivity			2	2			1	1					
	Each Connection			2	2			1	1					
	R_{ij}			2.583	2.226			1.958	1.958					
	S_{ij}			0.267	0.700			0.895	0.895		3.724			
	s_{ij}			0.384	0.543			1.073	1.073			4.000		
	$S_{ij}-s_{ij}$			-0.117	0.157			-0.178	-0.178				-0.276	0.076
	$(S_{ij}-s_{ij})^2$			0.014	0.025			0.032	0.032	0.140				
2														
O(7)	Total Connectivity	2	2			1	1							
	Each Connection	2	2			1	1							
	Rij	2.168	2.200			2.142	2.142							
	Sij	0.819	0.751			0.878	0.878				4.896			
	sij	0.664	0.664			0.672	0.672					4.000		
	Sij-sij	0.155	0.087			0.207	0.207						0.896	0.803
	(Sij-sij)2	0.024	0.008			0.043	0.043			0.148				
2														
O(8)	Total Connectivity			1	1									
	Each Connection			1	1									
	Rij			2.098	2.148									
	Sij			0.989	0.864						1.853			
	sij			0.921	1.079							2.000		
	Sij-sij			0.069	-0.215								-0.147	0.021
	(Sij-sij)2			0.005	0.046					0.051				
1														
										1.236				
	$\sum_i(S_{ij}-s_{ij})^2$	0.117	0.084	0.038	0.120	0.219	0.219	0.219	0.219	1.236				
	$V_j=\sum_i S_{ij}$	3.096	2.961	2.942	2.878	2.770	2.770	5.797	5.797					
	$z_j=\sum_i s_{ij}$	3.000	3.000	3.000	3.000	3.000	3.000	6.000	6.000					
	V_j-z_j	0.096	-0.039	-0.058	-0.122	-0.230	-0.230	-0.203	-0.203					
	$(V_j-z_j)^2$	0.009	0.002	0.003	0.015	0.053	0.053	0.041	0.041	0.218				1.575

Figure S1. Experimental and Calculated X-ray Powder Diffraction Patterns for $Bi_6Te_2O_{15}$.

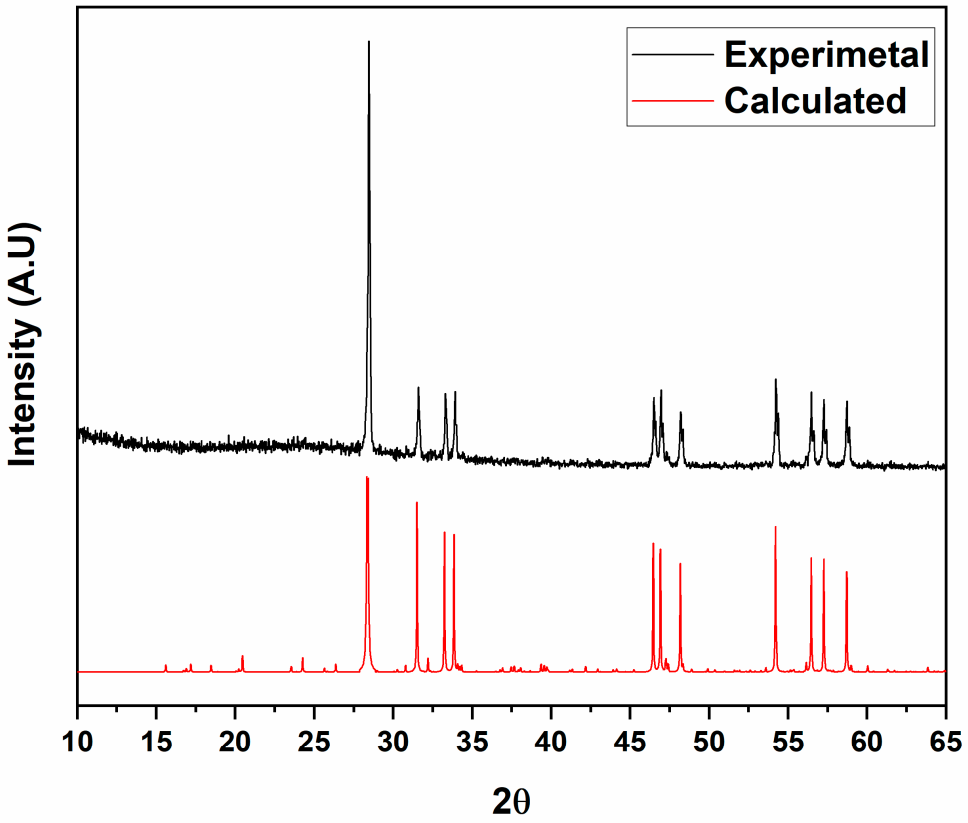
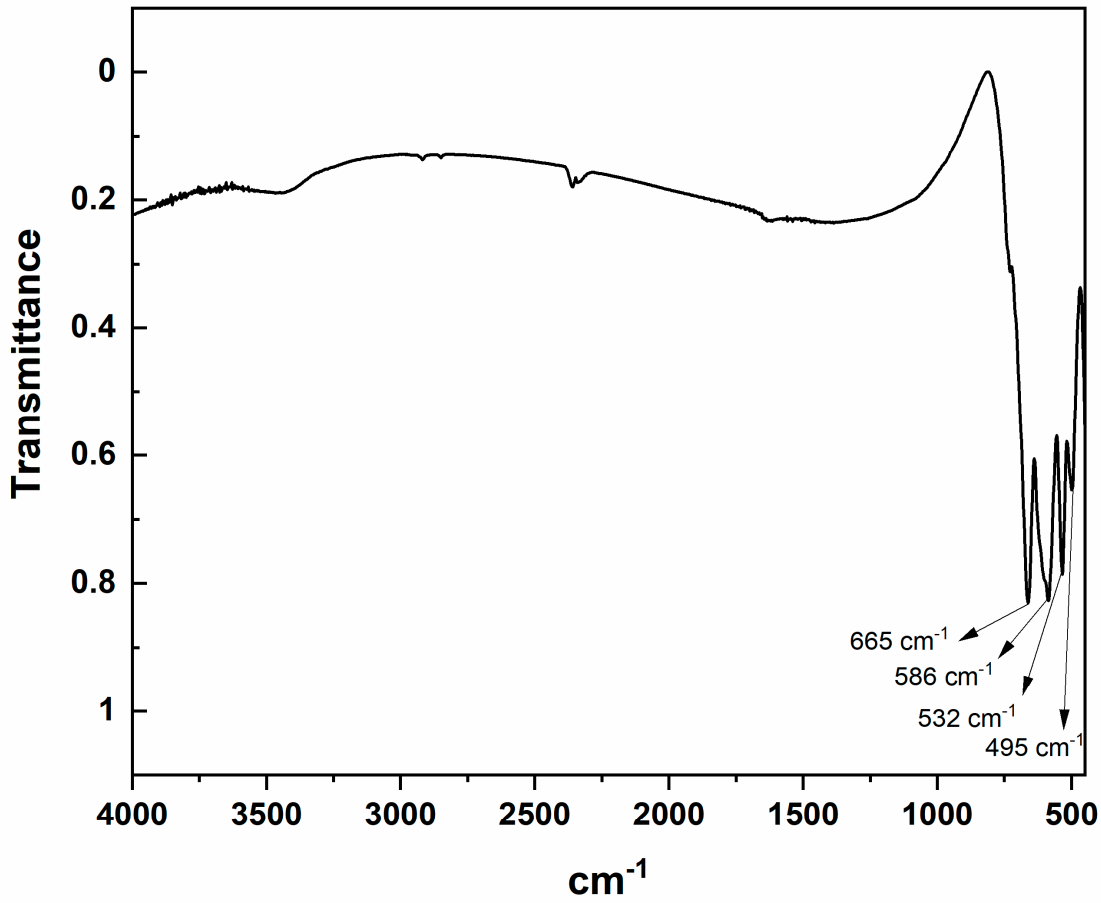


Figure S2. FT-IR Spectra of $Bi_6Te_2O_{15}$.



$Bi_6Te_2O_{15}$	
υ(Bi-O)	**υ(Te-O)**
532	665
495	586

Figure S3. Thermogravimetric analysis (TGA) diagram for $Bi_6Te_2O_{15}$.

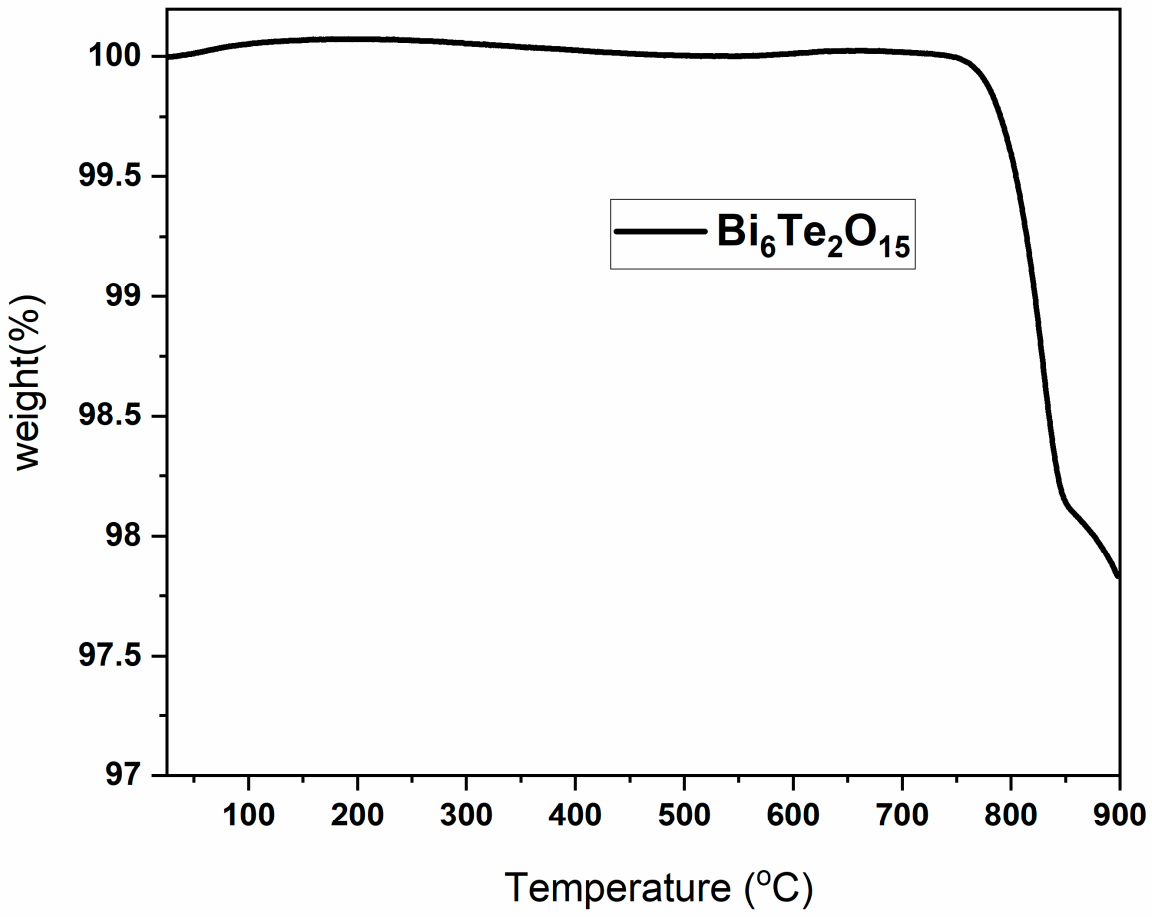


Figure S4. Powder XRD pattern for final residuals after TGA experiment

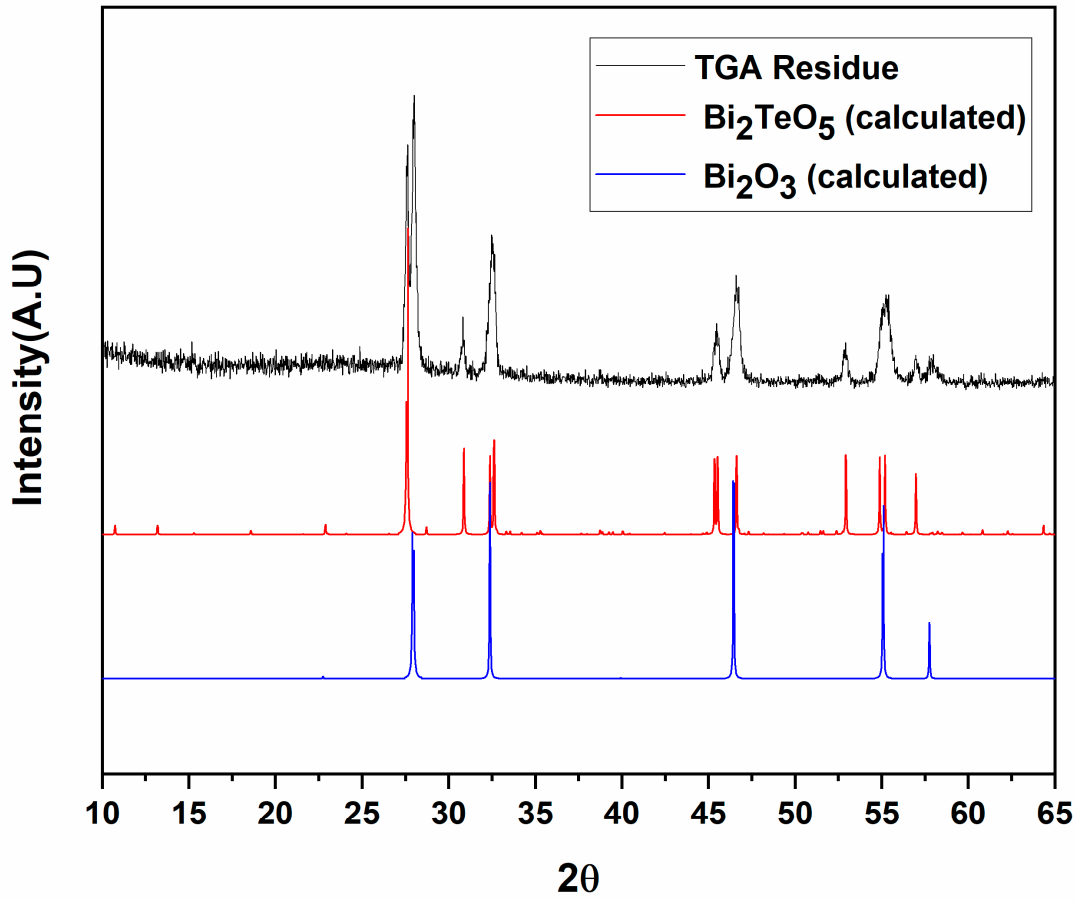


Figure S5. Dependence of total energy *versus* the unit cell volume by selected potential

(a) within GGA-PBE potential (b) within GGA-PBESol (c) within GGA-WC, respectively.

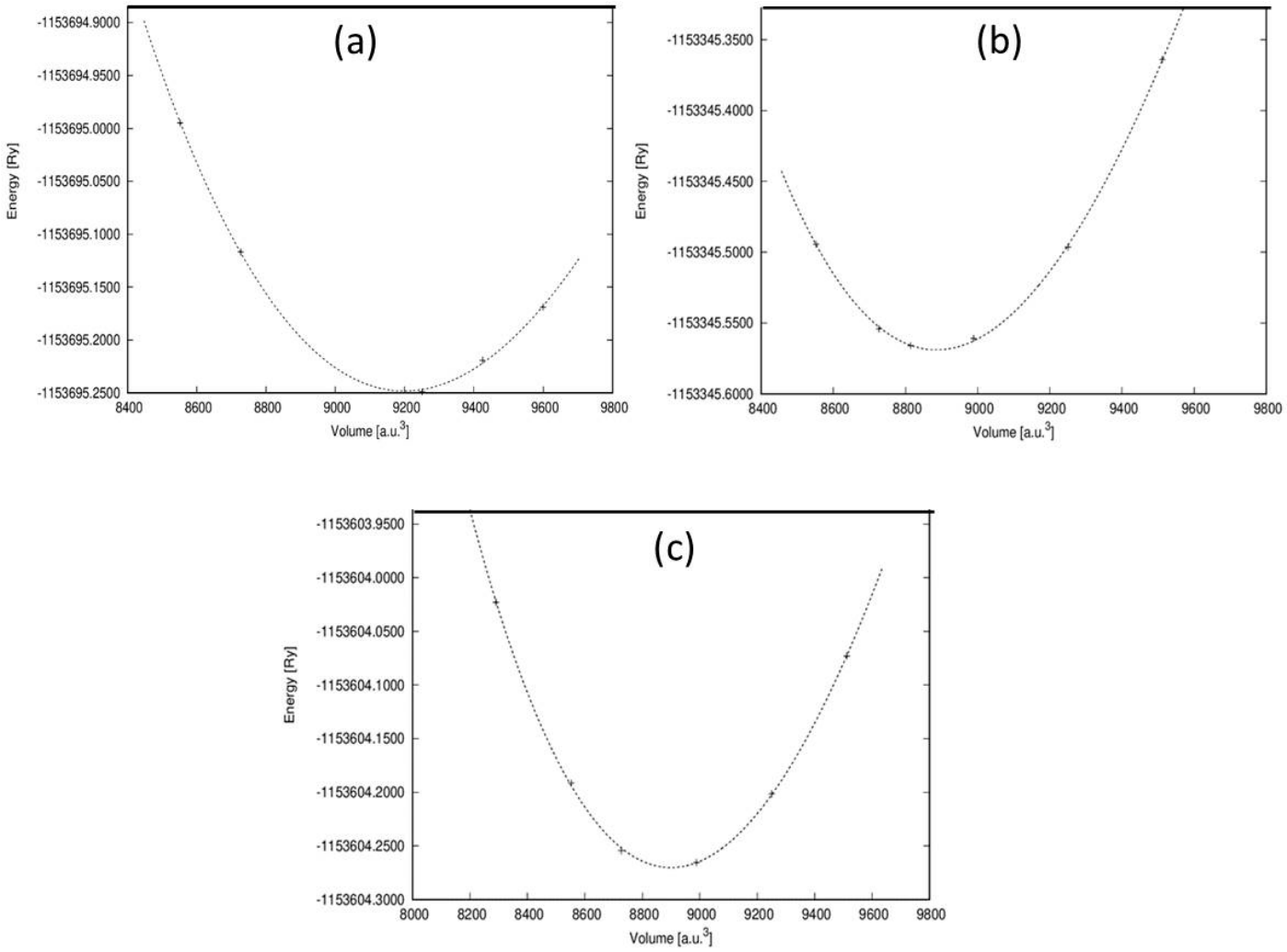


Figure S6. Other optical properties

Reflectivity R(ω), Optical conductivity σ(Ω·cm)$^{-1}$, Electron loss function L(ω), and Extinction coefficient k(ω) are depicted.