

Status Primary QM: Indexed Pressure/Temperature: Ambient Chemical Formula: Ba<sub>2</sub>TeO<sub>5</sub>  
 Structural Formula: 2 Ba O · Te O<sub>2</sub> Empirical Formula: Ba<sub>2</sub>O<sub>5</sub>Te Weight %: Ba56.95 O16.59 Te26.46  
 Atomic %: Ba25.00 O62.50 Te12.50 Compound Name: Barium Tellurate

Radiation: CuKα1 λ: 1.5406 Å Filter: Ni Beta Intensity: Diffractometer

SYS: Tetragonal SPGR: P41212 (92)

Author's Cell [ AuthCell a: 11.52 Å AuthCell c: 7.41 Å AuthCell Vol: 983.38 Å<sup>3</sup> AuthCell Z: 8.00

AuthCell MolVol: 122.92 ] Author's Cell Axial Ratio [ c/a: 0.643 ]

Density [ Dcalc: 6.515 g/cm<sup>3</sup> Dmeas: 6.39 g/cm<sup>3</sup> SS/FOM: F(30) = 14.3(0.024, 87)

Temp: 298.0 K (Ambient temperature assigned by ICDD editor)

Space Group: P41212 (92) Molecular Weight: 482.26

Crystal Data [ XtlCell a: 11.520 Å XtlCell b: 11.520 Å XtlCell c: 7.410 Å XtlCell α: 90.00°

XtlCell β: 90.00° XtlCell γ: 90.00° XtlCell Vol: 983.38 Å<sup>3</sup> XtlCell Z: 8.00 ]

Crystal Data Axial Ratio [ c/a: 0.643 a/b: 1.000 c/b: 0.643 ]

Reduced Cell [ RedCell a: 7.410 Å RedCell b: 11.520 Å RedCell c: 11.520 Å RedCell α: 90.00°

RedCell β: 90.00° RedCell γ: 90.00° RedCell Vol: 983.38 Å<sup>3</sup> ]

Crystal (Symmetry Allowed): Non-centrosymmetric - Enantiomorphic, Optical Activity, Piezo (2nd Harm.)

Subfile(s): Inorganic Pearson Symbol: tP64.00 Entry Date: 09/01/1975

#### References:

Type	DOI	Reference
Primary Reference		Natansohn. J. Electrochem. Soc. 120, 660 (1973).

Database Comments: Analysis: Chemical analysis: Ba(56.6%), Te(26.9). Warning: Lines with abs(delta 2Theta)>0.06 DEG.  
 Unit Cell Data Source: Powder Diffraction.

#### d-Spacings (37) - Ba<sub>2</sub>TeO<sub>5</sub> - 00-025-1470 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å

2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*
14.1816	6.240000	5	1	0	1		40.3767	2.232000	17	4	1	2		54.4403	1.684000	12	4	3	3	
15.3703	5.760000	6	2	0	0		40.9707	2.201000	16	5	0	1		55.0065	1.668000	10	3	0	4	
24.9919	3.560000	7	2	2	1		42.7377	2.114000	35	4	2	2		56.2514	1.634000	13	6	2	2	
25.2078	3.530000	20	1	0	2		43.5155	2.078000	5	3	0	3		56.8580	1.618000	7	5	4	2	
26.1103	3.410000	4	3	0	1		46.3577	1.957000	25	4	3	2		57.6358	1.598000	11	6	4	0	
27.8572	3.200000	100	3	2	0		47.2527	1.922000	8	6	0	0		59.2608	1.558000	5	4	0	4	
28.5865	3.120000	70	2	0	2		49.1543	1.852000	11	0	0	4		61.6603	1.503000	8	6	1	3	
29.6547	3.010000	45	2	1	2		51.1600	1.784000	7	4	4	2		63.3944	1.466000	6	6	2	3	
31.0151	2.881000	50	4	0	0		51.7828	1.764000	19	2	0	4		64.5258	1.443000	16	4	3	4	
32.6424	2.741000	25	2	2	2		52.3247	1.747000	10	5	4	1		66.7615	1.400000	6	5	2	4	
33.5745	2.667000	18	3	0	2		52.4863	1.742000	12	2	1	4		68.4798	1.369000	9	7	0	3	
36.8831	2.435000	8	4	2	1		53.3438	1.716000	17	6	3	0								
39.5632	2.276000	12	4	0	2		53.7496	1.704000	7	6	0	2								