Status Primary **Quality Mark:** Indexed **Environment:** Non-ambient Pressure **Temp:** 298.0 K **Pressure:** 18 GPa
Chemical Formula: Ba O **Empirical Formula:** Ba O **Weight %:** Ba89.57 O10.43 **Atomic %:** Ba50.00 O50.00
Compound Name: Barium Oxide **CAS Number:** 1304-28-5 **Entry Date:** 09/01/1976
Modification Date: 09/01/2003 **Modifications:** Quality

Radiation: MoKα1 (0.7093 Å) **Intensity:** Densiometer

Crystal System: Tetragonal **SPGR:** P4/nmm (129)
Author's Unit Cell [a: 4.397 Å **c:** 3.196 Å **Volume:** 61.79 Å³ **Z:** 2.00 **MolVol:** 30.89 **c/a:** 0.727 **]**
Calculated Density: 8.241 g/cm³ **SS/FOM:** F(13) = 31.9(0.0239, 17)

Space Group: P4/nmm (129) **Molecular Wt:** 153.33 g/mol
Crystal Data [a: 4.397 Å **b:** 4.397 Å **c:** 3.196 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **XtlCell Vol:** 61.79 Å³
XtlCell Z: 2.00 **c/a:** 0.727 **a/b:** 1.000 **c/b:** 0.727 **]**
Reduced Cell [a: 3.196 Å **b:** 4.397 Å **c:** 4.397 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **RedCell Vol:** 61.79 Å³ **]**

Crystal (Symmetry Allowed): Centrosymmetric

Subfiles: Inorganic, Metal & Alloy **Pearson Symbol:** tP4.00 **Prototype Structure (Formula Order):** Ba O
Prototype Structure (Alpha Order): Ba O **LPF Prototype Structure (Formula Order):** Ba O,tP4,129
LPF Prototype Structure (Alpha Order): Ba O,tP4,129 **ANX:** AX

Cross-Ref PDF #'s: 01-085-0418 (Primary), 04-002-2785 (Experimental <-> LPF), 04-007-1807 (Experimental <-> LPF)

References:

Type	DOI	Reference
Primary Reference	10.1063/1.1659673	Lin-gun Liu. J. Appl. Phys. 1971, 42, 3702.

Database Comments: Additional Patterns: See PDF 01-085-0418. ANX: AX. General Comments: Pressure at approximately 180 kbar. In Situ Condition: Powdered samples were placed in Bassett and Takahashi type diamond-anvil cell. NaCl was used to standardize pressure. Pressure was measured by length of spring. No pressure-transmitting medium was mentioned. Pressure of Datacollection: 18.0 GPa. Temperature of Data Collection: 298 K. Warning: Lines with abs(delta 2Theta)>0.06 DEG. Unit Cell Data Source: Powder Diffraction.

d-spacings (13) - Ba O - 00-026-0177 (Stick, Fixed Slit Intensity) - X-ray (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	*
27.857	**3.200**	55	0	0	1		50.255	1.814	20	2	0	1		70.783	1.330	10	3	0	1	
28.680	**3.110**	100	1	1	0		54.757	1.675	25	2	1	1		74.266	1.276	15	3	1	1	
34.617	2.589	40	1	0	1		59.429	1.554	25	2	2	0		76.954	1.238	30	2	1	2	
40.471	**2.227**	65	1	1	1		61.706	1.502	30	1	0	2								
41.029	2.198	10	2	0	0		67.032	1.395	20	2	2	1								