Status Primary **Quality Mark:** Star **Environment:** Ambient **Temp:** 298.0 K (Assigned by ICDD editor)
Chemical Formula: Ba C O3 **Empirical Formula:** Ba C O3 **Weight %:** Ba69.59 C6.09 O24.32
Atomic %: Ba20.00 C20.00 O60.00 **Compound Name:** Barium Carbonate **Mineral Name:** Witherite, syn
CAS Number: 14941-39-0 **Entry Date:** 09/01/1995

Radiation: CuKα1 (1.5406 Å) **Filter:** Ge Mono **Internal Standard:** Si **d-Spacing:** Diffractometer
Intensity: Diffractometer - Integrated

Crystal System: Orthorhombic **SPGR:** Pnma (62)
Author's Unit Cell [a: 6.4330(1) Å **b:** 5.3148(1) Å **c:** 8.9036(2) Å **Volume:** 304.42 Å³ **Z:** 4.00
MolVol: 76.11 **c/a:** 1.384 **a/b:** 1.210 **c/b:** 1.675 **]** **Calculated Density:** 4.306 g/cm³ **Color:** White
SS/FOM: F(30) = 255.1(0.0031, 38) **I/Ic:** 3.4

Space Group: Pnam (62) **Molecular Wt:** 197.33 g/mol
Crystal Data [a: 6.433 Å **b:** 8.904 Å **c:** 5.315 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **XtlCell Vol:** 304.42 Å³
XtlCell Z: 4.00 **c/a:** 0.826 **a/b:** 0.722 **c/b:** 0.597 **]**
Reduced Cell [a: 5.315 Å **b:** 6.433 Å **c:** 8.904 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **RedCell Vol:** 304.42 Å³ **]**

εα: =1.530 **nωβ:** =1.679 **εγ:** =1.680 **Sign:** =- **2V:** =9°(calc.)

Crystal (Symmetry Allowed): Centrosymmetric

Subfiles: Common Phase, Educational Pattern, Forensic, Inorganic, Mineral Related (Mineral, Synthetic), Superconducting Material (Superconductor Related Material)

Mineral Classification: Aragonite (group), carbonate (subgroup) **Pearson Symbol:** oP20.00
Prototype Structure (Formula Order): K N O3 **Prototype Structure (Alpha Order):** K N O3

Cross-Ref PDF #'s: 00-044-1487 (Alternate), 01-071-2394 (Primary), 04-001-7133 (Experimental <-> LPF), 04-002-0437 (Experimental <-> LPF), 04-007-6606 (Experimental <-> LPF)

References:

Type	DOI	Reference
Primary Reference		Kern, A., Geyer, A., Eysel, W., Miner.-Petrog. Inst., Univ. Heidelberg, Germany. ICDD Grant-in-Aid 1993.

Database Comments: Additional Patterns: To replace 00-044-1487. See PDF 01-071-2394. General Comments: 2è determination based on profile fit method (Split Pearson VII). Sample Preparation: "Ba C O3", Aldrich (99.98%).

d-spacings (83) - Ba C O3 - 00-045-1471 (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	*
19.438	4.56294	8	0	1	1		53.327	1.71651	<1	1	0	5		74.455	1.27323	<1	5	0	1	
19.927	4.45206	4	0	0	2		53.668	1.70641	3	0	2	4		75.656	1.25598	<1	0	3	5	
23.890	**3.72159**	100	1	1	1		54.285	1.68844	2	0	1	5		76.159	1.24893	5	1	4	2	
24.296	**3.66031**	50	1	0	2		54.672	1.67740	12	1	3	1		76.934	1.23826	4	5	1	1	
27.712	3.21640	20	2	0	0		55.688	1.64920	14	1	2	4		77.096	1.23607	3	5	0	2	
29.503	3.02510	6	2	0	1		56.283	1.63317	12	1	1	5		77.349	1.23266	5	1	3	5	
29.609	3.01451	2	1	1	2		57.236	1.60822	3	4	0	0		77.696	1.22802	2	2	4	0	
32.510	2.75184	4	2	1	0		57.760	1.59485	<1	1	3	2		78.710	1.21472	4	1	1	7	
33.217	2.69487	<1	1	0	3		58.249	1.58264	<1	4	0	1		79.723	1.20181	4	2	2	6	
33.702	2.65719	18	0	2	0		59.067	1.56264	6	3	2	2		81.186	1.18381	2	2	4	2	
34.074	2.62903	30	2	1	1		59.837	1.54436	2	3	0	4		81.480	1.18027	1	4	3	1	
34.365	2.60743	16	2	0	2		60.512	1.52874	3	2	3	1		82.819	1.16456	1	4	1	5	
34.586	2.59127	40	0	1	3		60.844	1.52119	7	0	3	3		83.694	1.15459	1	2	1	7	
37.964	2.36812	1	1	2	1		61.038	1.51682	5	4	1	1		84.268	1.14819	<1	5	2	1	
39.459	2.28177	12	0	2	2		61.226	1.51261	2	4	0	2		84.932	1.14090	<1	0	4	4	
40.490	2.22602	4	0	0	4		61.459	1.50743	3	2	2	4		86.582	1.12334	4	1	4	4	
41.976	**2.15059**	50	1	2	2		62.023	1.49507	3	2	1	5		86.839	1.12068	4	5	2	2	
42.960	2.10358	20	1	0	4		62.540	1.48395	3	0	0	6		87.504	1.11386	2	5	0	4	
44.170	2.04872	18	2	2	0		68.120	1.37535	12	2	3	3		88.374	1.10513	4	4	3	3	
44.881	2.01791	40	2	1	3		68.625	1.36646	10	4	1	3		89.239	1.09665	2	1	0	8	
46.397	1.95544	<1	1	1	4		69.733	1.34743	14	2	0	6		89.435	1.09475	3	3	4	2	
46.768	1.94079	30	3	1	1		70.463	1.33525	7	3	2	4		89.865	1.09063	2	4	0	6	
46.994	1.93198	14	3	0	2		70.866	1.32864	4	0	4	0		90.594	1.08374	2	3	3	5	
48.038	1.89241	1	1	2	3		70.991	1.32661	8	3	1	5		91.506	1.07530	1	2	4	4	
48.899	1.86108	6	2	2	2		71.743	1.31454	2	4	2	2		91.903	1.07169	3	3	1	7	
49.772	1.83046	3	2	0	4		72.444	1.30354	1	4	0	4		93.751	1.05537	<1	0	5	1	
50.189	1.81623	<1	3	1	2		72.958	1.29562	6	0	2	6		94.197	1.05154	<1	2	0	8	
52.629	1.73762	3	0	3	1		74.455	1.27323	<1	0	4	2								