Status Primary **Quality Mark:** Star **Environment:** Ambient **Temp:** 298.5 K **Chemical Formula:** Ba2 Cu3 Y O7
Empirical Formula: Ba2 Cu3 O7 Y **Weight %:** Ba41.23 Cu28.62 O16.81 Y13.35
Atomic %: Ba15.38 Cu23.08 O53.85 Y7.69 **Compound Name:** Barium Copper Yttrium Oxide **Entry Date:** 09/01/1988

Radiation: CuKα1 (1.5406 Å) **Filter:** Graph Mono **Internal Standard:** Si FP **d-Spacing:** Diffractometer
Cutoff: 17.70 Å **Intensity:** Diffractometer - Peak

Crystal System: Orthorhombic **SPGR:** Pmmm (47)
Author's Unit Cell [a: 3.8856(3) Å **b:** 11.6804(7) Å **c:** 3.8185(4) Å **Volume:** 173.30 Å³ **Z:** 1.00
MolVol: 173.30 **c/a:** 0.983 **a/b:** 0.333 **c/b:** 0.327 **]** **Calculated Density:** 6.383 g/cm³ **Color:** Black
SS/FOM: F(30) = 66.0(0.0091, 50)

Space Group: Pmmm (47) **Molecular Wt:** 666.19 g/mol
Crystal Data [a: 3.886 Å **b:** 11.680 Å **c:** 3.819 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **XtlCell Vol:** 173.30 Å³
XtlCell Z: 1.00 **c/a:** 0.983 **a/b:** 0.333 **c/b:** 0.327 **]**
Reduced Cell [a: 3.819 Å **b:** 3.886 Å **c:** 11.680 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **RedCell Vol:** 173.30 Å³ **]**

Crystal (Symmetry Allowed): Centrosymmetric

Subfiles: Common Phase, Inorganic, NBS Pattern, Superconducting Material (High Tc Superconductor)
Pearson Symbol: oP13.00 **ANX:** AB2C3X7

Cross-Ref PDF #'s: 04-002-0084 (Experimental <-> LPF), 04-002-2881 (Experimental <-> LPF), 04-002-2915 (Experimental <-> LPF), 04-002-2924 (Experimental <-> LPF), 04-002-2928 (Experimental <-> LPF), 04-002-2947 (Experimental <-> LPF), 04-002-2953 (Experimental <-> LPF), 04-002-2954 (Experimental <-> LPF), 04-002-2955 (Experimental <-> LPF), 04-002-2956 (Experimental <-> LPF), 04-002-2960 (Experimental <-> LPF), 04-002-2970 (Experimental <-> LPF), 04-002-2972 (Experimental <-> LPF), 04-002-6376 (Experimental <-> LPF), 04-002-8367 (Experimental <-> LPF), 04-002-8368 (Experimental <-> LPF), 04-002-8369 (Experimental <-> LPF), 04-002-8388 (Experimental <-> LPF), 04-002-8403 (Experimental <-> LPF), 04-002-8404 (Experimental <-> LPF), 04-002-8405 (Experimental <-> LPF), 04-002-8406 (Experimental <-> LPF), 04-005-5520 (Experimental <-> LPF), 04-005-8421 (Experimental <-> LPF), 04-005-8451 (Experimental <-> LPF), 04-006-5734 (Experimental <-> LPF), 04-006-5752 (Experimental <-> LPF), 04-006-5837 (Experimental <-> LPF), 04-006-6754 (Experimental <-> LPF), 04-006-6800 (Experimental <-> LPF), 04-006-6873 (Experimental <-> LPF), 04-006-6962 (Experimental <-> LPF), 04-006-7130 (Experimental <-> LPF), 04-006-7483 (Experimental <-> LPF), 04-006-7525 (Experimental <-> LPF), 04-006-7629 (Experimental <-> LPF), 04-006-7703 (Experimental <-> LPF), 04-006-7711 (Experimental <-> LPF), 04-006-7987 (Experimental <-> LPF), 04-007-4542 (Experimental <-> LPF), 04-007-4808 (Experimental <-> LPF), 04-009-7724 (Experimental <-> LPF), 04-009-7725 (Experimental <-> LPF)

References:

Type	DOI	Reference
Primary Reference		Wong-Ng, W., McMurdie, H., Paretzkin, B., Hubbard, C., Dragoo, A., NBS (USA). ICDD Grant-in-Aid 1987.
Structure		1. Siegrist, T., Sunshine, S., Murphy, D., Cava, R., Zahurak, S. Phys. Rev. B: Condens. Matter. Mater. Phys. 1987, 35, 7137.
Structure		2. Cava, R., Batlogg, R., van Dover, R., Murphy, D., Sunshine, S., Siegrist, T., Remeika, J., Rietman, E., Zahurak, S., Espinosa, G. Phys. Rev. Lett. 1987, 58, 1676.
Unit Cell		Wong-Ng, W., McMurdie, H., Paretzkin, B., Hubbard, C., Dragoo, A. Powder Diffr. 1987, 2, 192.

Database Comments: ANX: AB2C3X7. Analysis: The oxygen content was analyzed by differential thermal gravimetric analysis. General Comments: Superconductor with Tc of 92 K. Sample Preparation: The sample was obtained from F. Beech of the Reactor Radiation Division, NBS. A stoichiometric mixture of CuO, "Y2 O3" and "Ba C O3" were intimately mixed and fired at 773 K overnight. Reaction with container was avoided by placing the pellet on a support of the same material. The resulting powder was ground and pressed into pellets and refired at 1173 K overnight. The pellets were reground, pressed and fired at 1223 K overnight. Final annealing took place at 1023 K for 27 hours under oxygen. Structures: The sample was characterized by neutron Reitveld refinement technique by A. Santoro, at NBS. The compound was first reported by Cava and Batlogy. The structure was determined by Siearist, T. and Sunshine, S. et al. (1). Temperature of Data Collection: The temperature of data collection was 298.5 K. Unit Cell Data Source: Powder Diffraction.

d-spacings (63) - Ba2 Cu3 Y O7 - 00-038-1433 (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	*
7.557	11.68900	<1	0	1	0		27.553	3.23460	3	1	2	0	
15.169	5.83612	4	0	2	0		27.892	3.19605	5	0	2	1	
22.834	3.89125	10	0	3	0		30.617	2.91753	<1	0	4	0	
23.273	3.81884	4	0	0	1		32.537	**2.74962**	55	1	3	0	

2θ (°)	d (Å)	I	h	k	l	*
32.841	**2.72486**	100m	0	3	1	
33.756	2.65306	2	1	1	1	
36.369	2.46823	3	1	2	1	
38.511	2.33573	13m	0	5	0	
38.798	2.31911	5	0	4	1	
40.383	2.23167	14	1	3	1	
45.523	1.99093	2m	1	4	1	
46.632	1.94613	22	0	6	0	
46.724	1.94252	21	2	0	0	
47.579	1.90958	12	0	0	2	
51.494	1.77322	4	1	5	1	
52.525	1.74082	3	1	6	0	
52.732	1.73447	4	0	6	1	
53.399	1.71437	2	0	3	2	
54.995	1.66831	2	0	7	0	
55.312	1.65952	1	2	2	1	
58.205	**1.58371**	26	1	6	1	
58.825	1.56851	13	1	3	2	
60.307	1.53344	<1	1	7	0	
60.493	1.52919	1	0	7	1	
62.078	1.49388	2	2	5	0	
62.260	1.48995	2	2	4	1	
62.807	1.47828	3	0	5	2	
65.569	1.42254	2	1	7	1	
68.132	1.37514	5	2	6	0	
68.616	1.36661	5	1	8	0	
68.795	1.36349	13m	0	8	1	
68.887	1.36190	12	2	0	2	
72.818	1.29776	1	0	9	0	
72.993	1.29508	<1	3	0	0	
73.559	1.28651	2m	1	6	2	
74.975	1.26569	<1	2	7	0	
75.613	1.25658	1	0	7	2	
77.245	1.23406	<1	2	4	2	
77.478	1.23093	4	1	9	0	
77.652	1.22860	6	0	9	1	
77.824	1.22631	5	3	0	1	
79.085	1.20989	5m	0	3	3	
79.747	1.20151	3	2	7	1	
81.138	1.18438	1	1	2	3	
81.810	1.17635	2	2	5	2	
82.333	1.17020	<1	3	3	1	
82.496	1.16830	1	0	10	0	
83.647	1.15512	1	1	3	3	
87.025	1.11876	3	1	10	0	
87.284	1.11610	6m	2	8	1	
87.746	1.11142	4	1	8	2	
90.348	1.08605	1	3	5	1	
91.086	1.07916	1	2	9	0	
91.719	1.07336	1m	0	9	2	
93.024	1.06170	1	0	11	0	
93.783	1.05509	1	2	7	2	
95.850	1.03774	4	3	6	1	
96.390	1.03335	4	3	3	2	
97.142	1.02735	4	1	6	3	