Status Primary **Quality Mark:** Star **Environment:** Ambient **Temp:** 298.0 K (Assigned by ICDD editor)
Chemical Formula: Y2 O3 **Empirical Formula:** O3 Y2 **Weight %:** O21.26 Y78.74 **Atomic %:** O60.00 Y40.00
Compound Name: Yttrium Oxide **Mineral Name:** Yttriaite-(Y), syn **Alternate Name:** yttria **Entry Date:** 09/01/1991
Modification Date: 09/01/2002 **Modifications:** SpaceGroup

Radiation: CuKα1 (1.5406 Å) **Filter:** Graph Mono **Internal Standard:** Si **d-Spacing:** Diffractometer **Cutoff:** 15.00 Å
Intensity: Diffractometer - Peak

Crystal System: Cubic **SPGR:** Ia-3 (206)
Author's Unit Cell [a: 10.6041(5) Å **Volume:** 1192.40 Å³ **Z:** 16.00 **MolVol:** 74.53 **]**
Calculated Density: 5.031 g/cm³ **Avg. Melting Point:** 2713 K **Color:** White **SS/FOM:** F(30) = 160.0(0.0060, 31)
I/Ic: 9.1(8)

Space Group: Ia-3 (206) **Molecular Wt:** 225.81 g/mol
Crystal Data [a: 10.604 Å **b:** 10.604 Å **c:** 10.604 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00°
XtlCell Vol: 1192.40 Å³ **XtlCell Z:** 16.00 **a/b:** 1.000 **c/b:** 1.000 **]**
Reduced Cell [a: 9.183 Å **b:** 9.183 Å **c:** 9.183 Å **α:** 109.47° **β:** 109.47° **γ:** 109.47° **RedCell Vol:** 596.20 Å³ **]**

Crystal (Symmetry Allowed): Centrosymmetric

Subfiles: Ceramic (Semiconductor), Common Phase, Inorganic, Metal & Alloy, Mineral Related (Mineral, Synthetic), Superconducting Material

Mineral Classification: Bixbyite (group), Class Member **Pearson Symbol:** cI80.00
Prototype Structure (Formula Order): Mn Fe O3 **Prototype Structure (Alpha Order):** Fe Mn O3
LPF Prototype Structure (Formula Order): (Mn0.5 Fe0.5)2 O3,cI80,206
LPF Prototype Structure (Alpha Order): Fe Mn O3,cI80,206 **ANX:** A2X3

Cross-Ref PDF #'s: 00-025-1200 (Alternate), 00-063-0097 (Primary), 04-001-7256 (Experimental <-> LPF), 04-001-7709 (Experimental <-> LPF), 04-001-9349 (Experimental <-> LPF), 04-001-9554 (Experimental <-> LPF), 04-001-9891 (Experimental <-> LPF), 04-002-0039 (Experimental <-> LPF), 04-002-0143 (Experimental <-> LPF), 04-002-0197 (Experimental <-> LPF), 04-002-0293 (Experimental <-> LPF), 04-002-0302 (Experimental <-> LPF), 04-002-0315 (Experimental <-> LPF), 04-002-0434 (Experimental <-> LPF), 04-002-3916 (Experimental <-> LPF), 04-002-5170 (Experimental <-> LPF), 04-002-5312 (Experimental <-> LPF), 04-002-5376 (Experimental <-> LPF), 04-002-5640 (Experimental <-> LPF), 04-002-6197 (Experimental <-> LPF), 04-002-7545 (Experimental <-> LPF), 04-003-3337 (Experimental <-> LPF), 04-004-4336 (Experimental <-> LPF), 04-004-8961 (Experimental <-> LPF), 04-005-4269 (Experimental <-> LPF), 04-005-4378 (Experimental <-> LPF), 04-005-4779 (Experimental <-> LPF), 04-005-5073 (Experimental <-> LPF), 04-005-5119 (Experimental <-> LPF), 04-005-6550 (Experimental <-> LPF), 04-005-8060 (Experimental <-> LPF), 04-005-9640 (Experimental <-> LPF), 04-006-0197 (Experimental <-> LPF), 04-006-0976 (Experimental <-> LPF), 04-006-1998 (Experimental <-> LPF), 04-006-2010 (Experimental <-> LPF), 04-006-2207 (Experimental <-> LPF), 04-006-2298 (Experimental <-> LPF), 04-006-2304 (Experimental <-> LPF), 04-006-3683 (Experimental <-> LPF), 04-006-3684 (Experimental <-> LPF), 04-006-4365 (Experimental <-> LPF), 04-007-9716 (Experimental <-> LPF), 04-007-9751 (Experimental <-> LPF), 04-008-2590 (Experimental <-> LPF), 04-008-6362 (Experimental <-> LPF), 04-008-7447 (Experimental <-> LPF), 04-009-8404 (Experimental <-> LPF), 04-010-3289 (Experimental <-> LPF), 04-011-8012 (Experimental <-> LPF)

References:

Type	DOI	Reference
Primary Reference		Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA. ICDD Grant-in-Aid 1989.
Structure	10.2138/am.2011.3740	Mills, S., Kartashov, P., Ma, C., Rossman, G., Novgorodova, M., Kampf, A., Raudsepp, M. Am. Mineral. 2011, 96, 1166.

Database Comments: Additional Patterns: To replace 00-025-1200. See PDF 00-063-0097. ANX: A2X3. General Comments: Average relative standard deviation in intensity of the ten strongest reflections for three specimen mounts = 2%. Validated by a calculated pattern. Melting Point: 2713 K. Sample Preparation: Annealed for 48 hours at 1200 C. Sample Source or Locality: Sample obtained from Research Chemicals, Phoenix, Arizona, USA. Unit Cell Data Source: Single Crystal.

d-spacings (61) - Y2 O3 - 00-041-1105 (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	*
16.691	5.3070	<1	2	0	0		33.783	2.6510	24	4	0	0		41.694	2.1645	1	4	2	2	
20.494	4.3300	13	2	1	1		35.906	2.4990	5	4	1	1		43.498	2.0788	8	4	3	1	
29.150	**3.0610**	100	2	2	2		37.908	2.3715	1	4	2	0		46.898	1.9357	2	5	2	1	
31.531	2.8350	<1	3	2	1		39.846	2.2605	6	3	3	2		48.540	**1.8740**	39	4	4	0	

2θ (°)	d (Å)	I	h	k	l	*
50.128	1.8183	2	4	3	3	
51.666	1.7677	<1	6	0	0	
53.210	1.7200	5	6	1	1	
54.697	1.6767	1	6	2	0	
56.173	1.6361	4	5	4	1	
57.620	**1.5984**	25	6	2	2	
59.040	1.5633	5	6	3	1	
60.440	1.5304	4	4	4	4	
61.820	1.4995	2	5	4	3	
63.178	1.4705	1	6	4	0	
64.526	1.4430	3	7	2	1	
65.858	1.4170	1	6	4	2	
69.776	1.3467	2	6	5	1	
71.059	1.3255	4	8	0	0	
72.337	1.3052	3	8	1	1	
73.600	1.2859	2	8	2	0	
74.856	1.2674	2	6	5	3	
76.111	1.2496	1	6	6	0	
77.346	1.2327	3	8	3	1	
78.588	1.2163	6	6	6	2	
79.811	1.2007	<1	7	5	2	
81.037	1.1856	4	8	4	0	
82.256	1.1711	1	8	3	3	
83.481	1.1570	1	8	4	2	
84.694	1.1435	2	9	2	1	
85.900	1.1305	<1	6	6	4	
87.118	1.1178	2	8	5	1	
89.534	1.0938	2	9	3	2	
90.748	1.0823	4	8	4	4	
91.957	1.0712	2	9	4	1	
93.172	1.0604	1	10	0	0	
94.378	1.0500	1	10	1	1	
95.586	1.0399	3	10	2	0	
96.808	1.0300	1	9	4	3	
98.030	1.0204	3	10	2	2	
99.250	1.0111	2	10	3	1	
101.711	0.9932	2	8	7	1	
102.963	0.9845	2	10	4	0	
104.195	0.9762	1	10	3	3	
105.451	0.9680	2	10	4	2	
106.699	0.9601	1	9	5	4	
109.231	0.9448	2	11	2	1	
110.515	0.9374	1	8	8	0	
113.117	0.9231	1	10	4	4	
114.474	0.9160	1	11	3	2	
115.798	0.9093	1	10	6	0	
117.146	0.9027	1	11	4	1	
118.499	0.8963	2	10	6	2	
119.943	0.8897	<1	9	6	5	