00-047-0065 Dec 4, 2021 3:36 PM (XRD)

Status Primary **Quality Mark:** Star **Environment:** Ambient **Temp:** 298.0 K (Assigned by ICDD editor)
Chemical Formula: Pr Fe O3 **Empirical Formula:** Fe O3 Pr **Weight %:** Fe22.82 O19.61 Pr57.57
Atomic %: Fe20.00 O60.00 Pr20.00 **Compound Name:** Iron Praseodymium Oxide **Entry Date:** 09/01/1997

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

Crystal System: Orthorhombic **SPGR:** Pbnm (62)
Author's Unit Cell [a: 5.484(1) Å **b:** 5.5787(1) Å **c:** 7.7879(2) Å **Volume:** 238.26 Å³ **Z:** 4.00
MolVol: 59.56 **c/a:** 1.420 **a/b:** 0.983 **c/b:** 1.396 **]** **Calculated Density:** 6.823 g/cm³ **Color:** Dark reddish brown
SS/FOM: F(30) = 154.4(0.0061, 32)

Space Group: Pnma (62) **Molecular Weight:** 244.75 g/mol
Crystal Data [a: 5.579 Å **b:** 7.788 Å **c:** 5.484 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **XtlCell Vol:** 238.26 Å³
XtlCell Z: 4.00 **c/a:** 0.983 **a/b:** 0.716 **c/b:** 0.704 **]**
Reduced Cell [a: 5.484 Å **b:** 5.579 Å **c:** 7.788 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **RedCell Vol:** 238.26 Å³ **]**

Crystal (Symmetry Allowed): Centrosymmetric

Subfiles: Ceramic (Perovskite), Inorganic, Thermoelectric Material **Pearson Symbol:** oP 20.00
Prototype Structure [Formula Order]: Gd Fe O3 **Prototype Structure [Alpha Order]:** Fe Gd O3
LPF Prototype Structure [Formula Order]: Gd Fe O3,oP20,62
LPF Prototype Structure [Alpha Order]: Fe Gd O3,oP20,62

Cross-Ref PDF #'s: 00-015-0134 (Deleted)

References:

Type	DOI	Reference
Primary Reference		Parks, J., McCarthy, G., North Dakota State Univ., Fargo, ND, USA. ICDD Grant-in-Aid 1993.

Database Comments: Additional Patterns: To replace 00-015-0134. General Comments: Average relative standard deviation in intensity of the 10 strongest reflections for 3 specimen mounts = 1.6%. Trace impurity from starting materials present in sample. Validated with the aid of a calculated pattern. Sample Preparation: Prepared by firing "Pr6 O11" and "Fe2 O3" in a 1:3 molar ratio for 48 hours at 1200 C. Unit Cell Data Source: Powder Diffraction.

d-Spacings (81) - Pr Fe O3 - 00-047-0065 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å

2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*
19.79651	4.481000	1	1	0	1		58.08127	1.586800	23m	3	1	2	
22.73525	3.908000	20	1	1	0		59.09811	1.561900	2	2	2	3	
22.83591	3.891000	15	0	0	2		60.51832	1.528600	<1	3	2	0	
25.47186	3.494000	9	1	1	1		61.35705	1.509700	<1	2	3	1	
32.06529	**2.789000**	24	0	2	0		61.89792	1.497800	<1	1	0	5	
32.42351	**2.759000**	100	1	1	2		63.81730	1.457300	3	1	3	3	
32.63013	**2.742000**	29	2	0	0		64.31594	1.447200	1	1	1	5	
34.11464	2.626000	5	0	2	1		64.50070	1.443500	<1	3	1	3	
36.10004	2.486000	<1	1	2	0		67.04863	1.394700	1	0	4	0	
36.47960	2.461000	<1	2	1	0		67.88156	1.379600	9	2	2	4	
37.96595	2.368000	<1	1	2	1		68.26400	1.372800	3	0	4	1	
38.31884	2.347000	3m	1	0	3		68.38305	1.370700	3	4	0	0	
38.31884	2.347000	3m	2	1	1		69.00247	1.359900	<1	0	2	5	
39.70862	2.268000	8	0	2	2		69.50448	1.351300	<1	1	4	0	
40.18884	2.242000	11	2	0	2		70.70319	1.331300	<1m	1	4	1	
41.72378	2.163000	3	1	1	3		70.70319	1.331300	<1m	4	1	0	
43.12304	2.096000	1	1	2	2		71.17060	1.323700	<1	2	3	3	
43.47156	2.080000	<1	2	1	2		71.40684	1.319900	<1	1	2	5	
46.39030	1.955700	21	2	2	0		71.64479	1.316100	<1	2	1	5	
46.59966	1.947400	10	0	0	4		71.87183	1.312500	<1m	0	4	2	
47.82569	1.900300	6	0	2	3		71.87183	1.312500	<1m	4	1	1	
47.92752	1.896500	5	2	2	1		72.28576	1.306000	<1	1	3	4	
50.80594	1.795600	<1	1	2	3		72.43992	1.303600	<1	3	3	0	
51.07717	1.786700	1	2	1	3		72.80244	1.298000	1	0	0	6	
51.87756	1.761000	<1	1	3	0		72.91981	1.296200	2	3	1	4	
52.31178	1.747400	3	2	2	2		73.12293	1.293100	1	4	0	2	
52.45712	1.742900	4	1	1	4		73.61284	1.285700	2	3	3	1	
52.63918	1.737300	2	3	1	0		76.58035	1.243100	1	2	4	0	
53.28688	1.717700	7	1	3	1		77.09357	1.236100	3	3	3	2	
54.05124	1.695200	1	3	1	1		77.42010	1.231700	7	1	1	6	
57.37667	1.604600	9	1	3	2		77.52465	1.230300	5	4	2	0	
57.69506	1.596500	9	0	2	4		77.71212	1.227800	3	2	4	1	
58.08127	1.586800	23m	2	0	4		78.44151	1.218200	1	2	2	5	

2θ (°)	d (Å)	I	h	k	l	*
78.66487	1.215300	1	4	2	1	
81.13669	1.184400	<1m	2	4	2	
81.13669	1.184400	<1m	4	1	3	
81.79709	1.176500	<1	0	2	6	
82.07658	1.173200	1m	2	0	6	
82.07658	1.173200	1m	4	2	2	
82.65075	1.166500	2	1	3	5	
82.78922	1.164900	2	3	3	3	
83.26048	1.159500	<1	3	1	5	
85.59028	1.133800	1	0	4	4	
86.80772	1.121000	3m	2	4	3	
86.80772	1.121000	3m	4	0	4	
87.70790	1.111800	1	4	2	3	
89.66907	1.092500	<1	4	3	1	
89.81535	1.091100	<1	3	2	5	