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Tripraseodymium pentairon(III) dodecaoxide, $Pr_3Fe_5O_{12}$: a synchrotron radiation study

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Key indicators: single-crystal synchrotron study; T = 298 K; mean σ(Pr–Fe) = 0.000 Å; R factor = 0.019; wR factor = 0.021; data-to-parameter ratio = 550.1.

The title compound, pentairon tripraseodymium dodecaoxide (PrIG), has an iron garnet structure. There are two Fe site symmetries. One of the Fe atoms is coordinated by six O atoms, forming a slightly distorted octahedron, and has $\overline{3}$ site symmetry. The other Fe atom is coordinated by four O atoms, forming a slightly distorted tetrahedron, and has $\overline{4}$ site symmetry. FeO_6 octahedra and FeO_4 tetrahedra are linked together by corners. The Pr atom is coordinated by eight O atoms, forming a distorted dodecahedron, and has 222 site symmetry. The O atoms occupy the general positions.

Related literature

The title compound is isotypic with the $Ia\overline{3}d$ form of $Y_3Fe_5O_{12}$ (YIG). For related structures, see: Bonnet *et al.* (1975). For details of the crystal growth from low-temperature liquid-phase epitaxy, see: Fratello *et al.* (1986). For the extinction correction, see: Becker & Coppens (1975). X-ray intensities were measured avoiding multiple diffraction, see: Takenaka *et al.* (2008).

Experimental

Crystal data

$Pr_3Fe_5O_{12}$
M_r = 893.98
Cubic, $Ia\overline{3}d$
a = 12.6302 (3) Å
V = 2014.79 (8) Å^3
Z = 8
Synchrotron radiation
λ = 0.67171 Å
μ = 17.41 mm^{-1}
T = 298 K
0.035 mm (radius)

Data collection

Rigaku AFC four-circle diffractometer
Absorption correction: for a sphere [transmission coefficients for spheres tabulated in *International Tables C* (1992), Table 6.3.3.3, were interpolated with Lagrange's method (four-point interpolation; Yamauchi *et al.*, 1965)]
T_{min} = 0.413, T_{max} = 0.441
9351 measured reflections
1728 independent reflections
1728 reflections with $F > 3\sigma(F)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.021
S = 1.06
9351 reflections
17 parameters
$\Delta\rho_{max}$ = 2.52 e Å^{-3}
$\Delta\rho_{min}$ = −3.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pr1—O1	2.42410 (10)	Fe1—O1	2.03220 (10)
Pr1—O1^{i}	2.54010 (10)	Fe2—O1^{ii}	1.87450 (10)
O1—Fe1—O1^{i}	85.87 (1)	O1^{ii}—Fe2—O1^{iv}	100.02 (1)
O1^{ii}—Fe2—O1^{iii}	114.39 (1)		

Symmetry codes: (i) z, x, y; (ii) $x+\frac{1}{2}, y, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{4}, z-\frac{1}{4}, y+\frac{1}{4}$; (iv) $x+\frac{1}{2}, -y, z$.

Data collection: *AFC-5*, specially designed for PF-BL14A (Rigaku, 1984) and *IUANGLE* (Tanaka *et al.*, 1994); cell refinement: *RSLC-3 UNICS* system (Sakurai & Kobayashi, 1979); data reduction: *RDEDIT* (Tanaka, 2008); program(s) used to solve structure: *QNTAO* (Tanaka *et al.*, 2008); program(s) used to refine structure: *QNTAO*; molecular graphics: *ATOMS for Windows* (Dowty, 2000); software used to prepare material for publication: *RDEDIT*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2121).

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supplementary materials

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Tripraseodymium pentairon(III) dodecaoxide, $Pr_3Fe_5O_{12}$: a synchrotron radiation study

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Comment

The title compound, $Pr_3Fe_5O_{12}$ (PrIG), was difficult to be grown. It was grown by the low-temperature-liquid-phase epitaxy for the first time by Fratello *et al.* (1986). Though the crystal structure was assumed as iron-garnet-type structure by lattice constant and extinction rule, the complete structure was not determined. In this paper, we determine the O atom position and the complete structure by the full matrix least-squares program QNTAO. Since the R-factor is small and the residual density has no significant peaks where no atoms exists, the structure was finally determined to be iron-garnet structure. It is isotypic with the Ia$\bar{3}$d form of $Y_3Fe_5O_{12}$ (YIG). (Bonnet *et al.*, 1975). The Pr atom is coordinated by eight oxygen atoms. It forms a distorted dodecahedron. There are two Fe site symmetries. One of the Fe atom is coordinated by six oxygen atoms. It forms a slitely distorted octahedron. The other Fe atom is coordinated by four oxygen atoms. It forms a slightly distorted tetrahedron. FeO_6 octahedron and FeO_4 tetrahedron are linked together by corners. The structure of PrIG is drawn in Fig.1. And displacement ellipsoids of PrO_8 is drawn in Fig.2.

Experimental

Single crystals of praseodymium iron garnet were prepared by low temperature liquid phase epitaxy on $Sm_3(ScGa)_5O_{12}$ seeds with lattice parameters near the projected values for PrIG.

Refinement

X-ray intensities were measured avoiding multiple diffraction. (Takenaka *et al.*, 2008).

Figures

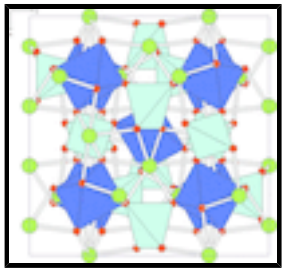

Fig. 1. The structure of $Pr_3Fe_5O_{12}$. Small red and large green spheres represent O and Pr atoms, respectively. Purple octahedron and blue tetrahedron represent FeO_6 and FeO_4 units, respectively.

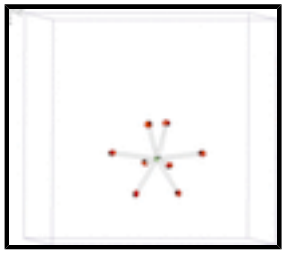

Fig. 2. View of PrO_8 with displacement ellipsoids at the 90% probability level. Green and red ellipsoids represent Pr and O atoms, in Fig.1.

Pentairon tripraseodymium dodecaoxide

Crystal data

$Pr_3Fe_5O_{12}$	D_x = 5.894 Mg m^{-3}
M_r = 893.98	Synchrotron radiation, λ = 0.67171 Å
Cubic, $Ia\bar{3}d$	Cell parameters from 9 reflections
Hall symbol: -I 4bd 2c 3	θ = 17.5–52.3°
a = 12.6302 (3) Å	μ = 17.41 mm^{-1}
V = 2014.79 (8) Å^3	T = 298 K
Z = 8	Sphere, black
F(000) = 3224	0.04 mm (radius)

Data collection

Rigaku AFC four-circle diffractometer	1728 independent reflections
Si 111	1728 reflections with $F > 3\sigma(F)$
Detector resolution: 1.25 × 1.25° pixels mm^{-1}	R_{int} = 0.016
ω/2θ scans	θ_{max} = 68.3°, θ_{min} = 3.7°
Absorption correction: for a sphere [Transmission coefficients for spheres tabulated in International Tables C (1992), Table 6.3.3.3, were interpolated with Lagrange's method (four-point interpolation (Yamauchi *et al.*, 1965)]	h = −9→34
T_{min} = 0.413, T_{max} = 0.441	k = −9→32
9351 measured reflections	l = −9→34

Refinement

Refinement on F	Primary atom site location: isomorphous structure methods
Least-squares matrix: full	Weighting scheme based on measured s.u.'s
$R[F^2 > 2\sigma(F^2)]$ = 0.019	$(\Delta/\sigma)_{max}$ = 0.003
$wR(F^2)$ = 0.021	$\Delta\rho_{max}$ = 2.52 e Å^{-3}
S = 1.06	$\Delta\rho_{min}$ = −3.16 e Å^{-3}
9351 reflections	Extinction correction: B–C type 1 Gaussian isotropic (Becker & Coppens, 1975)
17 parameters	Extinction coefficient: 0.255 (5)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Pr1	0.125000	0.000000	0.250000	0.00531 (1)
Fe1	0.000000	0.000000	0.000000	0.00512 (1)
Fe2	0.375000	0.000000	0.250000	0.00533 (1)
O1	−0.029622 (2)	0.052553 (2)	0.149166 (2)	0.00711 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00406 (2)	0.00594 (2)	0.00594 (2)	0	0	0.00111 (1)
Fe1	0.00512 (2)	0.00512 (2)	0.00512 (2)	−0.00023 (1)	−0.00023 (1)	−0.00023 (1)
Fe2	0.00411 (3)	0.00594 (2)	0.00594 (2)	0	0	0
O1	0.00718 (8)	0.00829 (8)	0.00587 (7)	−0.00004 (6)	0.00080 (6)	0.00038 (6)

Geometric parameters (Å, °)

Pr1—O1	2.42410 (10)	Fe1—O1^{i}	2.03220 (10)
Pr1—O1^{i}	2.54010 (10)	Fe1—O1^{viii}	2.03220 (10)
Pr1—O1^{ii}	2.42410 (10)	Fe1—O1^{ix}	2.03220 (10)
Pr1—O1^{iii}	2.54010 (10)	Fe1—O1^{x}	2.03220 (10)
Pr1—O1^{iv}	2.42410 (10)	Fe1—O1^{xi}	2.03220 (10)
Pr1—O1^{v}	2.54010 (10)	Fe2—O1^{xii}	1.87450 (10)
Pr1—O1^{vi}	2.42410 (10)	Fe2—O1^{iv}	1.87450 (10)
Pr1—O1^{vii}	2.54010 (10)	Fe2—O1^{xiii}	1.87450 (10)
Fe1—O1	2.03220 (10)	Fe2—O1^{vi}	1.87450 (10)
O1—Pr1—O1^{i}	67.75 (1)	O1—Fe1—O1^{viii}	85.87 (1)
O1—Pr1—O1^{ii}	72.66 (1)	O1—Fe1—O1^{ix}	180.00
O1—Pr1—O1^{iii}	124.91 (1)	O1—Fe1—O1^{x}	94.13 (1)
O1—Pr1—O1^{iv}	111.18 (1)	O1—Fe1—O1^{xi}	94.13 (1)
O1—Pr1—O1^{v}	73.25 (1)	O1^{xii}—Fe2—O1^{vi}	114.39 (1)
O1—Pr1—O1^{vi}	159.51 (1)	O1^{xii}—Fe2—O1^{iv}	114.39 (1)
O1—Pr1—O1^{vii}	95.43 (1)	O1^{xii}—Fe2—O1^{xiii}	100.02 (1)
O1—Fe1—O1^{i}	85.87 (1)		

Symmetry codes: (i) *z*, *x*, *y*; (ii) *x*, −*y*, −*z*+1/2; (iii) *z*, −*x*, −*y*+1/2; (iv) −*x*+1/4, −*z*+1/4, −*y*+1/4; (v) −*z*+1/4, −*y*+1/4, −*x*+1/4; (vi) −*x*+1/4, *z*−1/4, *y*+1/4; (vii) −*z*+1/4, *y*−1/4, *x*+1/4; (viii) *y*, *z*, *x*; (ix) −*x*, −*y*, −*z*; (x) −*z*, −*x*, −*y*; (xi) −*y*, −*z*, −*x*; (xii) *x*+1/2, *y*, −*z*+1/2; (xiii) *x*+1/2, −*y*, *z*.

Fig. 1

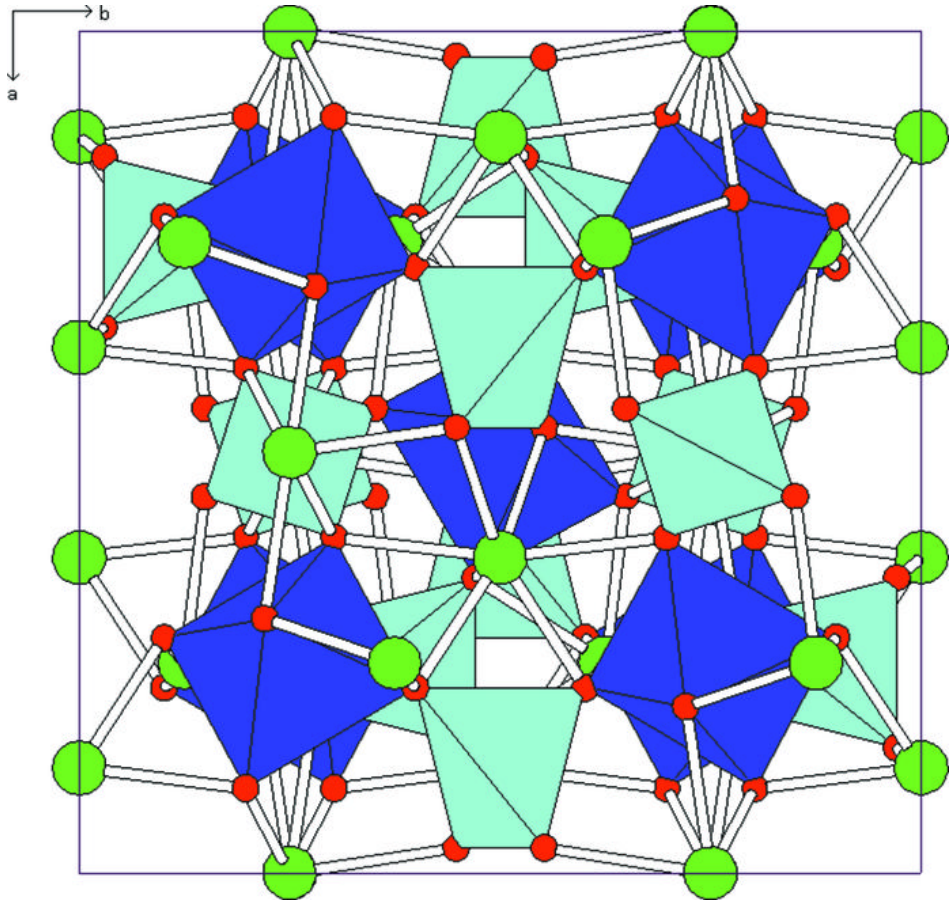

Fig. 2