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Trineodymium(III) pentairon(III) dodecaoxide, $Nd_3Fe_5O_{12}$

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Key indicators: single-crystal synchrotron study; T = 298 K; mean σ(Fe–O) = 0.0001 Å; R factor = 0.016; wR factor = 0.018; data-to-parameter ratio = 50.4.

The title compound, $Nd_3Fe_5O_{12}$ (NdIG), has an iron garnet structure. One of the Fe atoms is coordinated by six O atoms in a slightly distorted octahedral geometry and has $\bar{3}$ site symmetry. The other Fe atom is coordinated by four O atoms in a slightly distorted tetrahedral geometry and has $\bar{4}$ site symmetry. The FeO_6 octahedron and FeO_4 tetrahedron are linked together by corners. The Nd atom is coordinated by eight O atoms in a distorted dodecahedral geometry and has 222 site symmetry. The O atoms occupy general positions.

Related literature

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

Experimental

Crystal data

$Nd_3Fe_5O_{12}$
M_r = 903.97
Cubic, $Ia\bar{3}d$
a = 12.6128 (2) Å
V = 2006.48 (6) Å^3
Z = 8
Synchrotron radiation
λ = 0.67171 Å
μ = 18.30 mm^{-1}
T = 298 K
0.025 mm (radius)

Data collection

Rigaku AFC four-circle diffractometer
Absorption correction: spherical [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} = 0.502, T_{max} = 0.527
6653 measured reflections
1159 independent reflections
1159 reflections with $F > 3\sigma(F)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.018
S = 1.42
6653 reflections
23 parameters
$\Delta\rho_{max}$ = 1.61 e Å^{-3}
$\Delta\rho_{min}$ = −1.75 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Nd1—O1	2.41820 (10)	Fe1—O1	2.03300 (10)
Nd1—O1^{i}	2.52960 (10)	Fe2—O1^{ii}	1.87550 (10)
O1—Fe1—O1^{i}	85.59 (1)	O1^{ii}—Fe2—O1^{iv}	99.87 (1)
O1^{ii}—Fe2—O1^{iii}	114.47 (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 Corporation, 1984) and *IUANGLE* (Tanaka *et al.*, 1994).; cell refinement: *RSLC-3* (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* (Tanaka *et al.*, 2008); 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: BR2118).

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supporting information

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Trineodymium(III) pentairon(III) dodecaoxide, $Nd_3Fe_5O_{12}$

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S1. Comment

The title compound, $Nd_3Fe_5O_{12}$ (NdIG), 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 Nd 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 with site symmetry $\bar{3}$. It forms a slightly distorted octahedron. The other Fe atom is coordinated by four oxygen atoms, site symmetry $\bar{4}$. It forms a slightly distorted tetrahedron. FeO_6 octahedron and FeO_4 tetrahedron are linked together by corners. The structure of NdIG is drawn in Fig.1. And displacement ellipsoids of NdO_8 is drawn in Fig.2.

S2. Experimental

Single crystals of neodymium 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 NdIG.

S3. Refinement

The Becker–Coppens type 1 Gaussian anisotropic extinction parameters were employed ($\times 10^{-4}$ seconds). z11 = 10.2 (5), z22 = 10 (2), z33 = 12 (2), z12 = 1(1), z13 = -0.5 (7), z23 = -1(1). X-ray intensities were measured avoiding multiple diffraction. (Takenaka *et al.*, 2008).

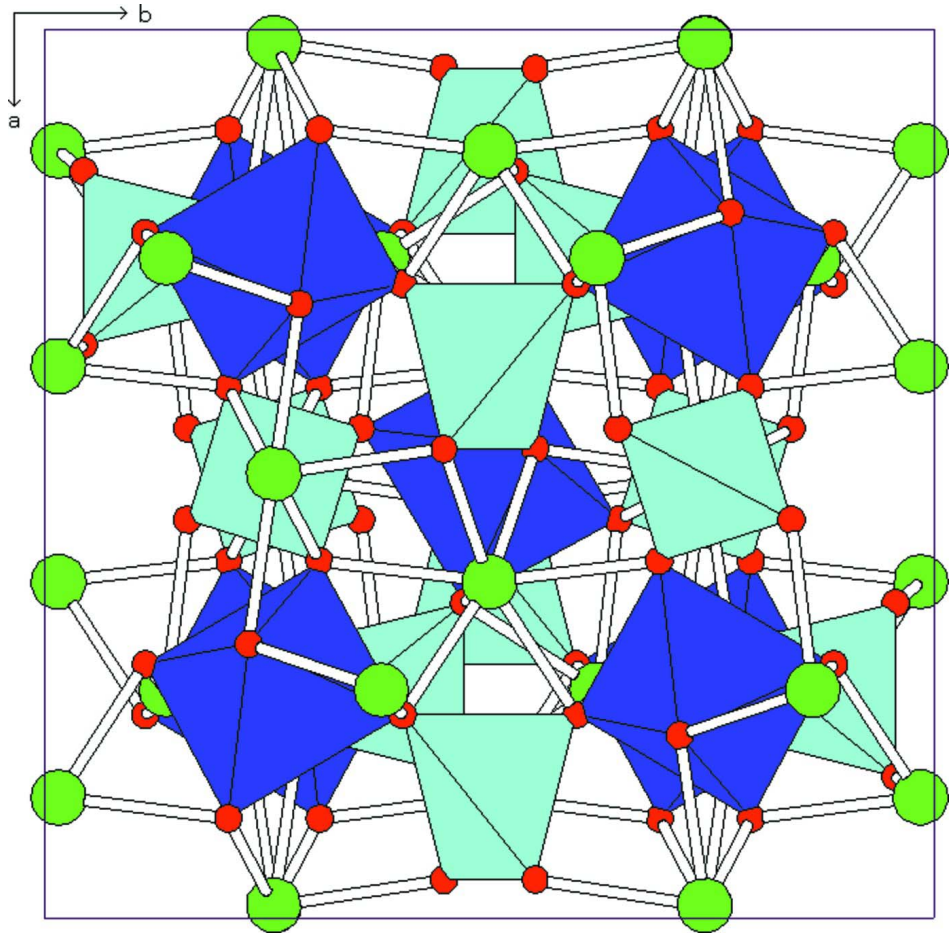

Figure 1

The structure of $Nd_3Fe_5O_{12}$. Small red and large green spheres represent O and Nd atoms, respectively. Purple octahedron and blue tetrahedron represent FeO_6 and FeO_4 units, respectively.

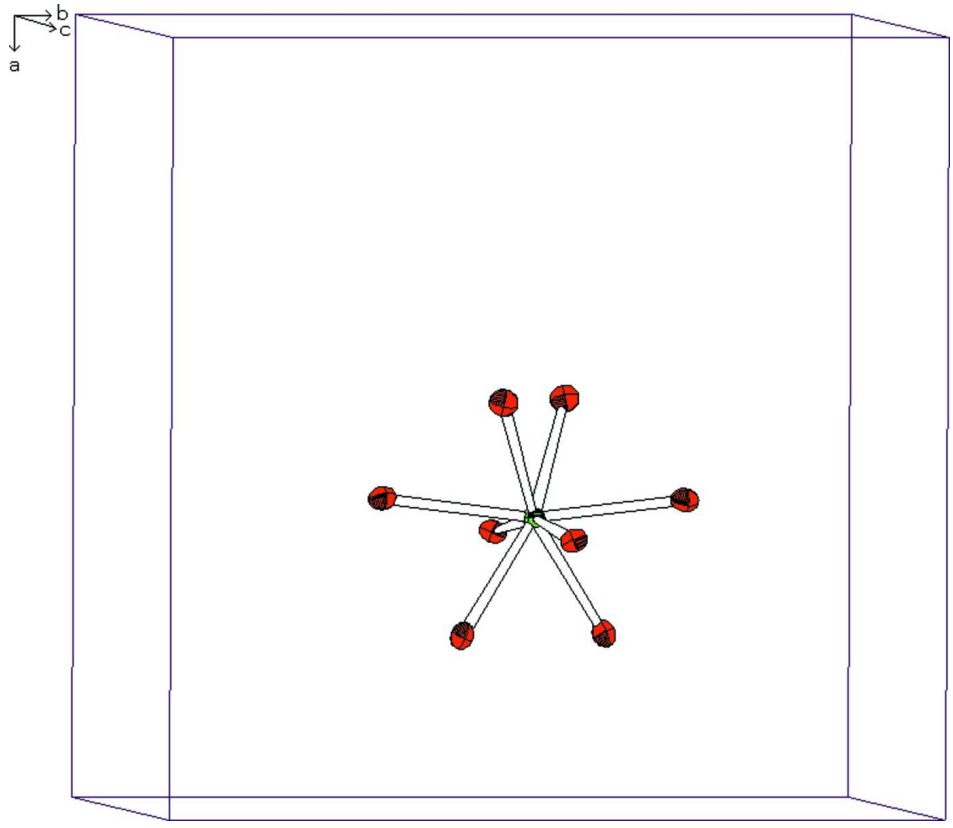

Figure 2

View of NdO_8 with displacement ellipsoids at the 90% probability level. Green and red ellipsoids represent Nd and O atoms, in Fig.1.

Trineodymium(III) pentairon(III) dodecaoxide

Crystal data

$Nd_3Fe_5O_{12}$
M_r = 903.97
Cubic, $Ia\bar{3}d$
Hall symbol: -I 4bd 2c 3
a = 12.6128 (2) Å
V = 2006.48 (6) Å^3
Z = 8
$F(000)$ = 3248
D_x = 5.985 Mg m^{-3}
Synchrotron radiation, λ = 0.67171 Å
Cell parameters from 24 reflections
θ = 35.7–42.4°
μ = 18.30 mm^{-1}
T = 298 K
Sphere, black
0.03 mm (radius)

Data collection

Rigaku AFC four-circle diffractometer
Si 111 monochromator
Detector resolution: 1.25×1.25 degrees pixels mm^{-1}
$\omega/2\theta$ scans
Absorption correction: for a sphere
Transmission coefficients for spheres tabulated in International Tables C (1992\bbr00), Table 6.3.3.3, were interpolated with Lagrange's method (four point interpolation; Yamauchi *et al.*, 1965).
T_{min} = 0.502, T_{max} = 0.527
6653 measured reflections
1159 independent reflections
1159 reflections with $F > 3\sigma(F)$
R_{int} = 0.017

θ_{max} = 53.9°, θ_{min} = 3.7°
h = −8→30
k = −8→30
l = −8→30

Refinement

Refinement on F
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.018
S = 1.42
6653 reflections
23 parameters
Primary atom site location: isomorphous structure methods
Weighting scheme based on measured s.u.'s
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 1.61 e Å^{-3}
$\Delta\rho_{min}$ = −1.75 e Å^{-3}
Extinction correction: (B-C type 1 Gaussian anisotropic; Becker & Coppens (1975)
Extinction coefficient: 0.308 (5)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Nd1	0.125000	0.000000	0.250000	0.00557 (1)
Fe1	0.000000	0.000000	0.000000	0.00501 (1)
Fe2	0.375000	0.000000	0.250000	0.00564 (1)
O1	−0.029295 (2)	0.053092 (2)	0.149342 (2)	0.00762 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.00421 (1)	0.00525 (1)	0.00525 (1)	0	0	0.00121 (1)
Fe1	0.00501 (2)	0.00501 (2)	0.00501 (2)	−0.00024 (2)	−0.00024 (2)	−0.00024 (2)
Fe2	0.00442 (3)	0.00625 (2)	0.00625 (2)	0	0	0
O1	0.00791 (8)	0.00880 (9)	0.00614 (7)	−0.00027 (7)	0.00102 (6)	0.00041 (7)

Geometric parameters (Å, º)

Nd1—O1	2.4182 (1)	Fe1—O1^{i}	2.0330 (1)
Nd1—O1^{i}	2.5296 (1)	Fe1—O1^{viii}	2.0330 (1)
Nd1—O1^{ii}	2.4182 (1)	Fe1—O1^{ix}	2.0330 (1)
Nd1—O1^{iii}	2.5296 (1)	Fe1—O1^{x}	2.0330 (1)
Nd1—O1^{iv}	2.4182 (1)	Fe1—O1^{xi}	2.0330 (1)
Nd1—O1^{v}	2.5296 (1)	Fe2—O1^{xii}	1.8755 (1)
Nd1—O1^{vi}	2.4182 (1)	Fe2—O1^{iv}	1.8755 (1)
Nd1—O1^{vii}	2.5296 (1)	Fe2—O1^{xiii}	1.8755 (1)
Fe1—O1	2.0330 (1)	Fe2—O1^{vi}	1.8755 (1)
O1—Nd1—O1^{i}	67.83 (1)	O1—Fe1—O1^{viii}	85.59 (1)
O1—Nd1—O1^{ii}	72.82 (1)	O1—Fe1—O1^{ix}	180.00
O1—Nd1—O1^{iii}	124.94 (1)	O1—Fe1—O1^{x}	94.41 (1)
O1—Nd1—O1^{iv}	110.91 (1)	O1—Fe1—O1^{xi}	94.41 (1)
O1—Nd1—O1^{v}	72.97 (1)	O1^{xii}—Fe2—O1^{vi}	114.47 (1)
O1—Nd1—O1^{vi}	159.79 (1)	O1^{xii}—Fe2—O1^{iv}	114.47 (1)

O1—Nd1—O1^{vii}	95.60 (1)	O1^{xii}—Fe2—O1^{xiii}	99.87 (1)
O1—Fe1—O1^{i}	85.59 (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*.