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# Trineodymium(III) pentairon(III) dodecaoxide, Nd<sub>3</sub>Fe<sub>5</sub>O<sub>12</sub>

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Key indicators: single-crystal synchrotron study;  $T = 298$  K; mean  $\sigma(\text{Fe}-\text{O}) = 0.0001$  Å;  $R$  factor = 0.016;  $wR$  factor = 0.018; data-to-parameter ratio = 50.4.

The title compound, Nd<sub>3</sub>Fe<sub>5</sub>O<sub>12</sub> (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<sub>6</sub> octahedron and FeO<sub>4</sub> 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<sub>3</sub>Fe<sub>5</sub>O<sub>12</sub> (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 <sub>3</sub> Fe <sub>5</sub> O <sub>12</sub>	Synchrotron radiation
$M_r = 903.97$	$\lambda = 0.67171$ Å
Cubic, $Ia\bar{3}d$	$\mu = 18.30$ mm <sup>-1</sup>
$a = 12.6128$ (2) Å	$T = 298$ K
$V = 2006.48$ (6) Å <sup>3</sup>	0.025 mm (radius)
$Z = 8$	

### Data collection

Rigaku AFC four-circle diffractometer	point interpolation; Yamauchi <i>et al.</i> , 1965)]
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	$T_{\min} = 0.502$ , $T_{\max} = 0.527$
	6653 measured reflections
	1159 independent reflections
	1159 reflections with $F > 3\sigma(F)$
	$R_{\text{int}} = 0.017$

### Refinement

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

**Table 1**

Selected geometric parameters (Å, °).

Nd1—O1	2.41820 (10)	Fe1—O1	2.03300 (10)
Nd1—O1 <sup>i</sup>	2.52960 (10)	Fe2—O1 <sup>ii</sup>	1.87550 (10)
O1—Fe1—O1 <sup>i</sup>	85.59 (1)	O1 <sup>ii</sup> —Fe2—O1 <sup>iv</sup>	99.87 (1)
O1 <sup>ii</sup> —Fe2—O1 <sup>iii</sup>	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*.

The authors thank Dr V. J. Fratello for supplying the crystals.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2118).

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**supplementary materials**

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## Trineodymium(III) pentairon(III) dodecaoxide, $\text{Nd}_3\text{Fe}_5\text{O}_{12}$

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### Comment

The title compound,  $\text{Nd}_3\text{Fe}_5\text{O}_{12}$  (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  $\text{Ia}\bar{3}\text{d}$  form of  $\text{Y}_3\text{Fe}_5\text{O}_{12}$  (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.  $\text{FeO}_6$  octahedron and  $\text{FeO}_4$  tetrahedron are linked together by corners. The structure of NdIG is drawn in Fig.1. And displacement ellipsoids of  $\text{NdO}_8$  is drawn in Fig.2.

### Experimental

Single crystals of neodymium iron garnet were prepared by low temperature liquid phase epitaxy on  $\text{Sm}_3(\text{ScGa})_5\text{O}_{12}$  seeds with lattice parameters near the projected values for NdIG.

### 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).

### Figures

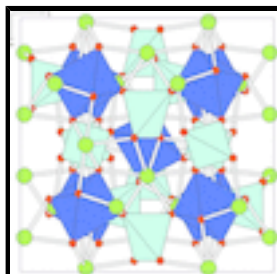


Fig. 1. The structure of  $\text{Nd}_3\text{Fe}_5\text{O}_{12}$ . Small red and large green spheres represent O and Nd atoms, respectively. Purple octahedron and blue tetrahedron represent  $\text{FeO}_6$  and  $\text{FeO}_4$  units, respectively.

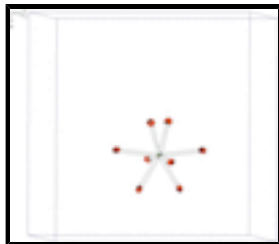


Fig. 2. View of NdO<sub>8</sub> with displacement ellipsoids at the 90% probability level. Green and red ellipsoids represent Nd and O atoms, in Fig. 1.

## Trineodymium(III) pentairon(III) dodecaoxide

### Crystal data

Nd <sub>3</sub> Fe <sub>5</sub> O <sub>12</sub>	$D_x = 5.985 \text{ Mg m}^{-3}$
$M_r = 903.97$	Synchrotron radiation, $\lambda = 0.67171 \text{ \AA}$
Cubic, $Ia\bar{3}d$	Cell parameters from 24 reflections
Hall symbol: -I 4bd 2c 3	$\theta = 35.7\text{--}42.4^\circ$
$a = 12.6128 (2) \text{ \AA}$	$\mu = 18.30 \text{ mm}^{-1}$
$V = 2006.48 (6) \text{ \AA}^3$	$T = 298 \text{ K}$
$Z = 8$	Sphere, black
$F(000) = 3248$	0.03 mm (radius)

### Data collection

Rigaku AFC four-circle diffractometer	1159 independent reflections
Si 111	1159 reflections with $F > 3\sigma(F)$
Detector resolution: $1.25 \times 1.25$ degrees pixels $\text{mm}^{-1}$	$R_{\text{int}} = 0.017$
$\omega/2\theta$ scans	$\theta_{\text{max}} = 53.9^\circ$ , $\theta_{\text{min}} = 3.7^\circ$
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 <i>et al.</i> , 1965).	$h = -8 \rightarrow 30$
$T_{\text{min}} = 0.502$ , $T_{\text{max}} = 0.527$	$k = -8 \rightarrow 30$
6653 measured reflections	$l = -8 \rightarrow 30$

### Refinement

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 ( $\text{\AA}$ ,  $^\circ$ )

Nd1—O1	2.41820 (10)	Fe1—O1 <sup>i</sup>	2.03300 (10)
Nd1—O1 <sup>i</sup>	2.52960 (10)	Fe1—O1 <sup>viii</sup>	2.03300 (10)
Nd1—O1 <sup>ii</sup>	2.41820 (10)	Fe1—O1 <sup>ix</sup>	2.03300 (10)
Nd1—O1 <sup>iii</sup>	2.52960 (10)	Fe1—O1 <sup>x</sup>	2.03300 (10)
Nd1—O1 <sup>iv</sup>	2.41820 (10)	Fe1—O1 <sup>xi</sup>	2.03300 (10)
Nd1—O1 <sup>v</sup>	2.52960 (10)	Fe2—O1 <sup>xii</sup>	1.87550 (10)
Nd1—O1 <sup>vi</sup>	2.41820 (10)	Fe2—O1 <sup>iv</sup>	1.87550 (10)
Nd1—O1 <sup>vii</sup>	2.52960 (10)	Fe2—O1 <sup>xiii</sup>	1.87550 (10)
Fe1—O1	2.03300 (10)	Fe2—O1 <sup>vi</sup>	1.87550 (10)
O1—Nd1—O1 <sup>i</sup>	67.83 (1)	O1—Fe1—O1 <sup>viii</sup>	85.59 (1)
O1—Nd1—O1 <sup>ii</sup>	72.82 (1)	O1—Fe1—O1 <sup>ix</sup>	180.00
O1—Nd1—O1 <sup>iii</sup>	124.94 (1)	O1—Fe1—O1 <sup>x</sup>	94.41 (1)
O1—Nd1—O1 <sup>iv</sup>	110.91 (1)	O1—Fe1—O1 <sup>xi</sup>	94.41 (1)
O1—Nd1—O1 <sup>v</sup>	72.97 (1)	O1 <sup>xii</sup> —Fe2—O1 <sup>vi</sup>	114.47 (1)
O1—Nd1—O1 <sup>vi</sup>	159.79 (1)	O1 <sup>xii</sup> —Fe2—O1 <sup>iv</sup>	114.47 (1)
O1—Nd1—O1 <sup>vii</sup>	95.60 (1)	O1 <sup>xii</sup> —Fe2—O1 <sup>xiii</sup>	99.87 (1)
O1—Fe1—O1 <sup>i</sup>	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)  $x+1/2, -y, z$ .

Fig. 1

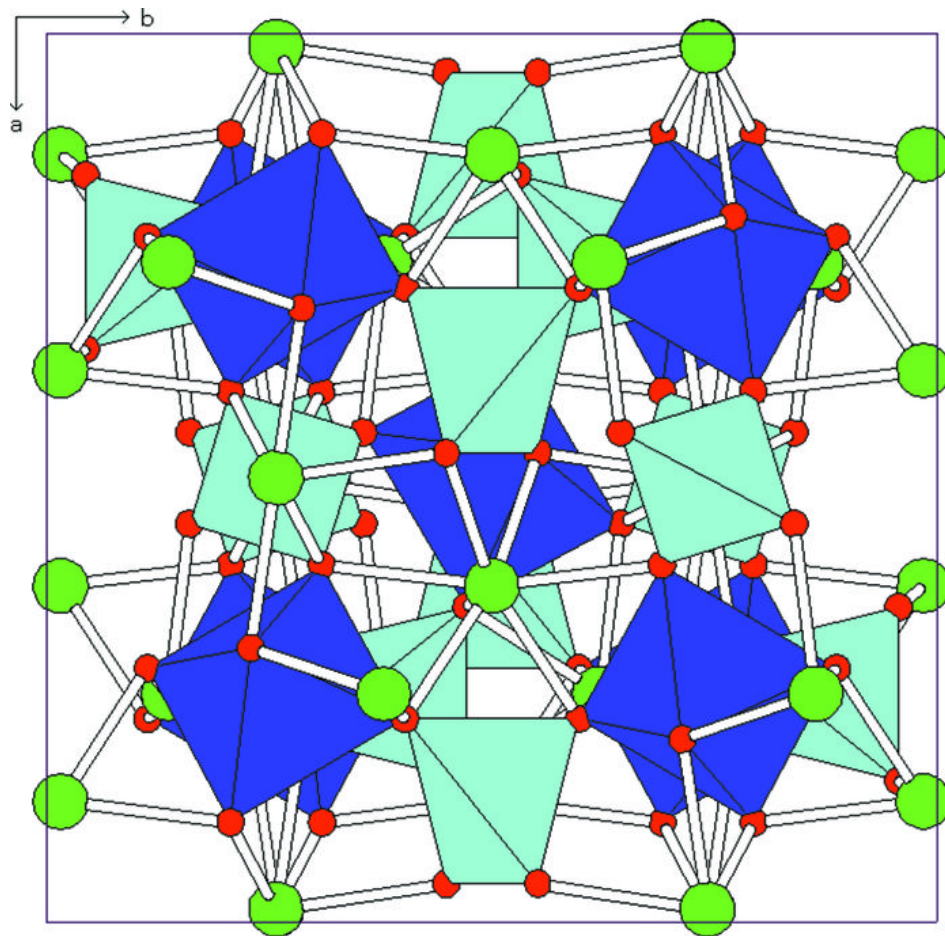


Fig. 2

