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Dineodymium(III) ditungstate(VI), $Nd_2W_2O_9$

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Key indicators: single-crystal X-ray study; T = 290 K; mean σ(W–O) = 0.007 Å; R factor = 0.037; wR factor = 0.093; data-to-parameter ratio = 19.6.

Single crystals of monoclinic $Nd_2W_2O_9$ were obtained by growth from tungsten borate flux in an atmosphere of air. The crystal structure consists of chains of distorted $[WO_6]$ octahedra that run along the c axis of the structure, and of $[NdO_9]$ polyhedra that are connected *via* common faces and common edges to form a three-dimensional framework.

Related literature

For literature on related structures, see: Lacorre *et al.* (2000), Goutenoire *et al.* (2000) and Evans *et al.* (2005) for $La_2Mo_2O_9$; Laligant *et al.* (2001) for $La_2W_2O_9$; Yoshimura *et al.* (1976) for $Ce_2W_2O_9$; Borisov & Klevtsova (1970) for $Pr_2W_2O_9$; Aruga *et al.* (2005) for $Eu_2W_2O_9$.

Experimental

Crystal data

$Nd_2W_2O_9$
M_r = 800.17
Monoclinic, $P2_1/c$
a = 7.6501 (11) Å
b = 9.8547 (10) Å
c = 9.2326 (13) Å
β = 107.538 (11)°
V = 663.69 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 49.96 mm^{-1}
T = 290 (1) K
0.25 × 0.15 × 0.13 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: numerical [*X-SHAPE* (Stoe & Cie, 1999) and *X-RED* (Stoe & Cie, 2001)] T_{min} = 0.080, T_{max} = 0.469
15723 measured reflections
2330 independent reflections
2072 reflections with $I > 2\sigma(I)$
R_{int} = 0.088

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
S = 1.09
2330 reflections
119 parameters
$\Delta\rho_{max}$ = 2.34 e Å^{-3}
$\Delta\rho_{min}$ = −1.62 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 2002); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2082).

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supporting information

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Dineodymium(III) ditungstate(VI), $Nd_2W_2O_9$

Peter Held and Petra Becker

S1. Comment

The crystal structure of the title compound consists of two symmetrically non-equivalent Nd atoms that both are ninefold coordinated by oxygen. Nd - O bond lengths range from 2.377 (6) Å to 3.096 (7) Å for Nd1 and from 2.447 (7) Å to 2.743 (8) Å for Nd2. (The distance to the next nearest cation, W1 in case of Nd1 with distance Nd1 - W1 = 3.3885 (7) Å, W2 in case of Nd2 with distance Nd2 - W2 = 3.3800 (7) Å, is taken as the limit of the first oxygen coordination surrounding of Nd). The [NdO_9] polyhedra can be described as distorted capped square antiprisms for both Nd atoms. The polyhedra of Nd1 are sharing edges, thus forming chains that run along the *a*-axis of the structure (Fig. 1). Parallel to the *a*-*c* plane of the structure these chains are linked by dimers of edge-sharing coordination polyhedra of Nd2 (groups [Nd_2O_{16}]). The polyhedra dimers of Nd2 and the polyhedra chains of Nd1 are connected *via* common faces (*i.e.* three common oxygen ligands) between a Nd2 polyhedron and a Nd1 polyhedron, and a common edge of the Nd2 polyhedron and an adjacent Nd1 polyhedron (for the atomic numbering scheme see Fig. 3). From this linkage sheets of [NdO_9] polyhedra parallel to the *a*-*c* plane result (Fig. 1). Along the *b*-axis the sheets are stacked in parallel with a translation of *c*/2, and are connected by common edges of Nd1 and Nd2 polyhedra alternatingly to neighbouring polyhedra sheets on both sides. This connection scheme results in a three-dimensional framework of [NdO_9] polyhedra with narrow channels along the *c*-axis, where tungsten atoms are located. Within the [NdO_9] polyhedra sheets Nd1 - Nd2 distances as short as 3.7787 (9) Å occur (face sharing of [NdO_9] polyhedra).

Between the [NdO_9] polyhedra sheets chains of distorted [WO_6] octahedra are running along the *c*-axis (see Fig. 1 and Fig. 2). The octahedra chains consist of pairs of edge-sharing [WO_6] units, each pair combining an octahedron [W1 O_6] and an octahedron [W2 O_6]. The octahedra pairs are connected *via* common corners O9 to infinite chains. W—O bonds to bridging oxygen atoms are elongated with bond lengths ranging from 1.855 (7) Å to 2.202 (7) Å. All oxygen atoms are simultaneously ligands of neodymium and of tungsten.

Borisov & Klevtsova (1970) published the structure of $Pr_2W_2O_9$, however, with rather large uncertainty of the oxygen positions. $Nd_2W_2O_9$ turns out to be isomorphous to this compound, but it should be noted that in $Pr_2W_2O_9$ the coordination of one of the Pr atoms was regarded as eightfold, only, while the other is ninefold coordinated, as both Nd atoms are in $Nd_2W_2O_9$. Due to this, in $Pr_2W_2O_9$ the Pr coordination polyhedra are not connected to sheets but only to stripes parallel to the *a*-*c* plane of the structure. The inclusion of nine oxygen atoms to the coordination surrounding of Nd1 in $Nd_2W_2O_9$ is meaningful, both, with respect to the connection scheme of Nd coordination polyhedra and regarding the Nd - O distances, where a distinct gap between distances of the nine oxygen atoms included in the coordination polyhedron and distances of further oxygen atoms is seen. All further oxygen atoms have distances Nd1 - O equal or larger than 3.4694 Å, which is more than the shortest Nd—W distance.

After the discovery of fast oxygen ion conduction in $La_2Mo_2O_9$ by Lacorre *et al.* (2000) interest in $RE_2M_2O_9$ (*RE* = rare earth element, *M* = Mo, W) compounds renewed. For La compounds $La_2M_2O_9$ (*M* = Mo, W) evidence for the occurrence of a high-temperature (space group $P2_13$) and a low-temperature modification (space group $P2_1$ for $La_2Mo_2O_9$, space group $P\bar{1}$ for $La_2W_2O_9$), together with their structure determination was given by Goutenoire *et al.* (2000), Laligant *et al.* (2001) and Evans *et al.* (2005); a similar polymorphy had been already presumed earlier for $Ce_2W_2O_9$ by Yoshimura *et al.* (1976). Recently, the compound $Eu_2W_2O_9$ was mentioned to be isomorphous to $Pr_2W_2O_9$ (and hence to $Nd_2W_2O_9$) by Aruga *et al.* (2005).

S2. Experimental

Light purple prismatic single crystals of $Nd_2W_2O_9$ were obtained by growth from tungsten borate flux using a melt of composition Nd_2O_3: B_2O_3: WO_3 = 22.5: 25: 52.5. An appropriate homogenized powder mixture of Nd_2O_3 (99.9%, Alfa Aesar), B_2O_3 (99.98% Alfa Aesar) and WO_3 (99.8%, Alfa Aesar) was heated in a covered platinum crucible in air atmosphere to 1423 K and subsequently cooled at a rate of 3 K h^{-1} to 1173 K. Transparent single crystals of the title compound were separated mechanically from the tungsten borate flux.

S3. Refinement

Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

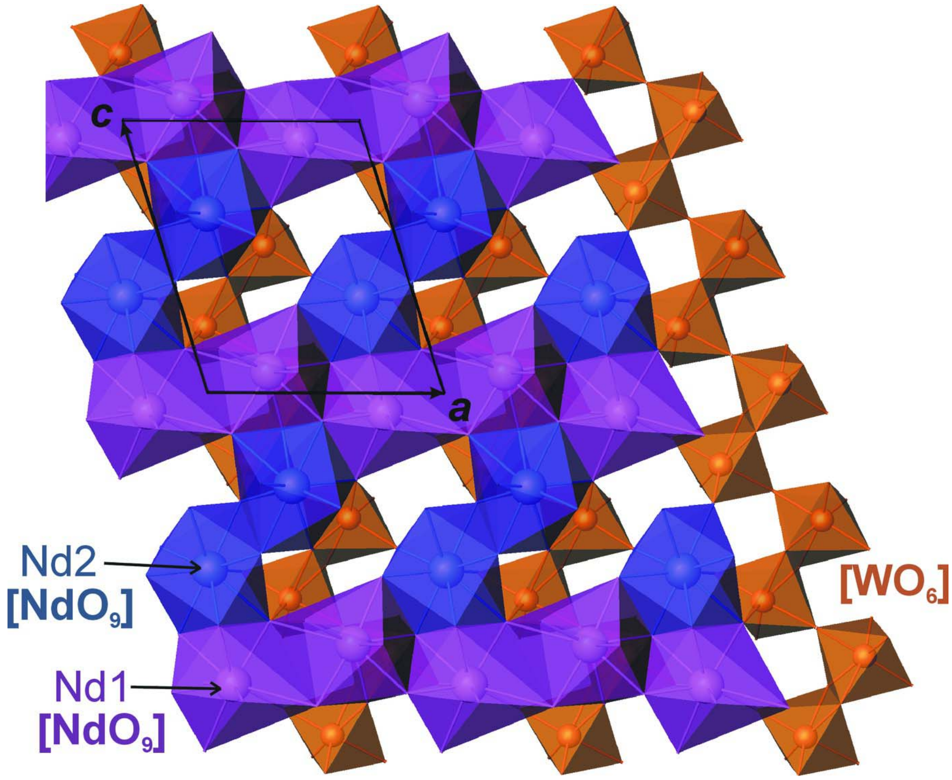

Figure 1

Projection along [010] of a fraction of the crystal structure of $Nd_2W_2O_9$, showing one sheet of [NdO_9] polyhedra that lies parallel to the *a-c* plane, and one layer of isolated chains of alternately edge- and corner-sharing [WO_6] octahedra. Large purple and violet spheres denote Nd1 and Nd2 atoms, respectively, smaller orange spheres denote W atoms. Oxygen atoms are indicated by the corners of the coordination polyhedra and are not drawn.

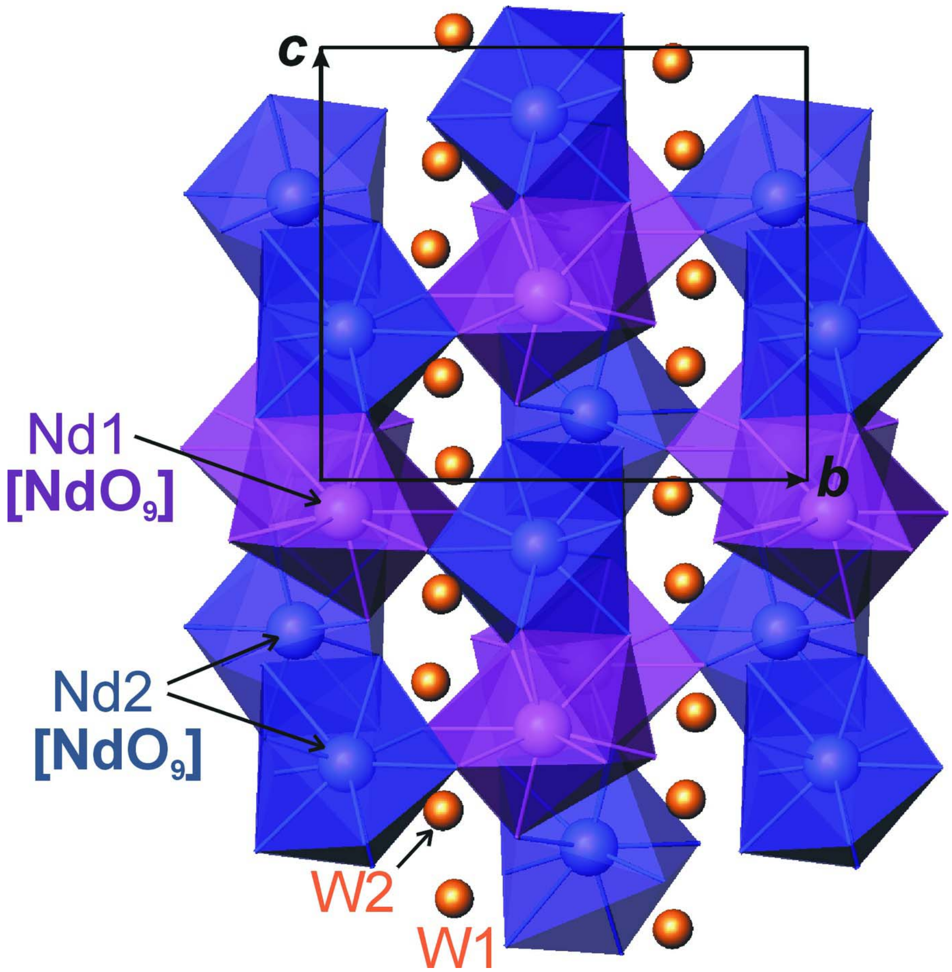

Figure 2

View of the structure of $Nd_2W_2O_9$ along the *a*-axis, emphasizing the arrangement and mutual connection of [NdO_9] polyhedra sheets that lie parallel to the *a*-*c* plane. Nd atoms are denoted by large purple and violet spheres. Tungsten atoms (marked with smaller orange spheres) occupy interstitial space between the sheets of Nd coordination polyhedra and are arranged in layers parallel to the *a*-*c* plane. Oxygen atoms are indicated by the corners of the coordination polyhedra and are not drawn.

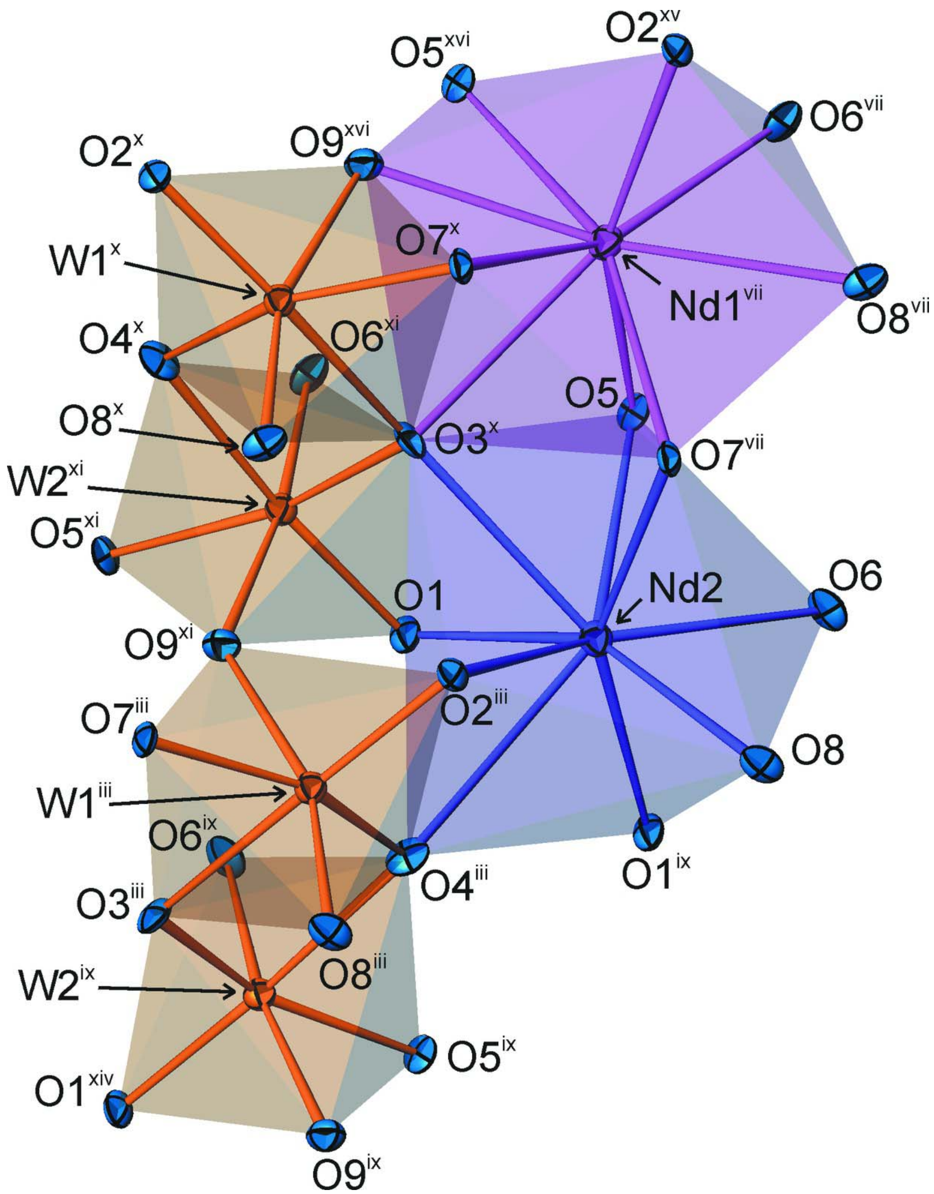

Figure 3

Fraction of the structure of $Nd_2W_2O_9$ with atomic numbering scheme (projection approximately along the *a*-axis). Coordination polyhedra are indicated as a guide for the eye. Atoms are drawn as 50% probability ellipsoids. (Symmetry codes: (iii) -*x* + 1, -*y* + 1, -*z*; (vii) *x*, -*y* + 3/2, *z* + 1/2; (ix) -*x*, -*y* + 1, -*z*; (*x*) -*x* + 1, *y* - 1/2, -*z* + 1/2; (xi) -*x*, *y* - 1/2, -*z* + 1/2; (xiv) *x*, -*y* + 1/2, *z* - 1/2; (xv) *x*, *y*, *z* + 1; (xvi) -*x*, -*y* + 1, -*z* + 1).

Dineodymium(III) ditungstate(VI)

Crystal data

$Nd_2W_2O_9$
M_r = 800.17
Monoclinic, $P2_1/c$
a = 7.6501 (11) Å
b = 9.8547 (10) Å
c = 9.2326 (13) Å
β = 107.538 (11)°
V = 663.69 (15) Å^3
Z = 4
F(000) = 1360
D_x = 8.008 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 25 reflections
$\theta = 20.1–27.6°$
$\mu = 49.96\ mm^{-1}$
$T = 290$ K
Prism, light purple
0.25 × 0.15 × 0.13 mm

Data collection

Stoe IPDSII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: numerical [*X-SHAPE* (Stoe & Cie, 1999) and *X-RED* (Stoe & Cie, 2001)]
$T_{min} = 0.080$, $T_{max} = 0.469$
15723 measured reflections
2330 independent reflections
2072 reflections with $I > 2\sigma(I)$
$R_{int} = 0.088$
$\theta_{max} = 32.2°$, $\theta_{min} = 2.8°$
$h = -11\rightarrow11$
$k = -14\rightarrow14$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.093$
$S = 1.09$
2330 reflections
119 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 16.1611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.34$ e Å^{-3}
$\Delta\rho_{min} = -1.62$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00391 (19)

Special details

Experimental. A suitable single-crystal was carefully selected under a polarizing microscope and mounted in a glass capillary. The scattering intensities were collected on an imaging plate diffractometer (*IPDS* II, Stoe & Cie) equipped with a fine focus sealed tube X-ray source (Mo Kα, $\lambda = 0.71073$ Å) operating at 50 kV and 30 mA. Intensity data for the title compound were collected at room temperature by ω-scans in 180 frames ($0 < \omega < 180°$; $\varphi = 0°$ and 90°, $\Delta\omega = 2°$, exposure time of 10 min) in the 2Θ range 2.29 to 59.53°. Structure solution and refinement were carried out using the programs *SIR92* (Altomare *et al.*, 1993) and *SHELXL97* (Sheldrick, 2008). A numerical absorption correction (*X-RED* (Stoe & Cie, 2001) was applied after optimization of the crystal shape (*X-SHAPE* (Stoe & Cie, 1999)). The last cycles of refinement included atomic positions and anisotropic parameters for all atoms. The final difference maps were free of any chemically significant features. The refinement was based on F^2 for ALL reflections.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	y	z	U_{iso}*/U_{eq}
W1	0.57359 (5)	0.72579 (4)	−0.03462 (4)	0.01073 (11)
W2	−0.07053 (5)	0.75136 (4)	0.26320 (4)	0.01058 (11)
Nd1	0.28098 (7)	0.95544 (5)	0.07401 (5)	0.01298 (13)
Nd2	0.22931 (7)	0.55245 (5)	0.15396 (5)	0.01243 (13)
O1	−0.0113 (10)	0.3795 (7)	0.0941 (7)	0.0131 (12)
O2	0.4920 (10)	0.5969 (7)	−0.1761 (7)	0.0144 (12)
O3	0.7367 (9)	0.8644 (7)	0.1417 (7)	0.0128 (12)
O4	0.7687 (10)	0.6210 (8)	0.0779 (8)	0.0152 (13)

O5	0.0438 (10)	0.5887 (7)	0.3447 (8)	0.0139 (12)
O6	0.0995 (10)	0.7810 (7)	0.1630 (8)	0.0149 (13)
O7	0.4449 (9)	0.8935 (6)	−0.1077 (7)	0.0109 (11)
O8	0.4091 (10)	0.7091 (8)	0.0739 (8)	0.0147 (12)
O9	−0.2605 (10)	0.6904 (8)	0.3610 (7)	0.0143 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
W1	0.01099 (18)	0.01014 (18)	0.01053 (17)	0.00011 (11)	0.00245 (12)	0.00011 (11)
W2	0.01064 (18)	0.01036 (17)	0.01018 (17)	0.00025 (11)	0.00230 (12)	0.00037 (11)
Nd1	0.0138 (2)	0.0122 (2)	0.0118 (2)	−0.00143 (15)	0.00216 (16)	0.00027 (15)
Nd2	0.0124 (2)	0.0116 (2)	0.0123 (2)	−0.00062 (15)	0.00227 (16)	0.00016 (15)
O1	0.016 (3)	0.009 (3)	0.011 (3)	0.002 (2)	−0.001 (2)	0.003 (2)
O2	0.022 (3)	0.010 (3)	0.009 (3)	−0.002 (2)	0.001 (2)	−0.003 (2)
O3	0.015 (3)	0.011 (3)	0.011 (3)	0.006 (2)	0.001 (2)	0.001 (2)
O4	0.013 (3)	0.017 (3)	0.012 (3)	0.006 (2)	−0.001 (2)	0.005 (2)
O5	0.018 (3)	0.009 (3)	0.012 (3)	0.002 (2)	0.001 (2)	0.004 (2)
O6	0.013 (3)	0.015 (3)	0.019 (3)	−0.004 (2)	0.008 (2)	0.004 (2)
O7	0.014 (3)	0.006 (3)	0.011 (3)	0.002 (2)	0.001 (2)	0.002 (2)
O8	0.011 (3)	0.019 (3)	0.016 (3)	−0.004 (2)	0.007 (2)	−0.001 (3)
O9	0.017 (3)	0.015 (3)	0.012 (3)	0.001 (2)	0.007 (2)	0.002 (2)

Geometric parameters (Å, º)

W1—O2	1.794 (7)	Nd1—Nd2^{vi}	3.7787 (9)
W1—O8	1.837 (7)	Nd1—Nd2^{viii}	3.9479 (9)
W1—O4	1.855 (7)	Nd2—O8	2.331 (7)
W1—O7	1.938 (6)	Nd2—O7^{vii}	2.379 (6)
W1—O9^{i}	1.990 (7)	Nd2—O1	2.447 (7)
W1—O3	2.202 (7)	Nd2—O6	2.473 (8)
W1—Nd1^{ii}	3.3885 (7)	Nd2—O1^{ix}	2.485 (6)
W1—Nd2^{iii}	3.4651 (7)	Nd2—O2^{iii}	2.548 (8)
W1—Nd1	3.5344 (7)	Nd2—O5	2.598 (7)
W2—O1^{iv}	1.796 (6)	Nd2—O3^{x}	2.601 (7)
W2—O6	1.833 (7)	Nd2—O4^{iii}	2.743 (8)
W2—O5	1.872 (6)	Nd2—W2^{xi}	3.3800 (7)
W2—O3^{v}	1.917 (6)	Nd2—W1^{iii}	3.4651 (7)
W2—O9	2.020 (7)	O1—W2^{xi}	1.796 (6)
W2—O4^{v}	2.196 (7)	O1—Nd2^{ix}	2.485 (6)
W2—Nd2^{iv}	3.3800 (7)	O2—Nd1^{vi}	2.439 (7)
W2—Nd2	3.3934 (7)	O2—Nd2^{iii}	2.548 (8)
Nd1—O5^{vi}	2.377 (6)	O3—W2^{xii}	1.917 (6)
Nd1—O9^{iv}	2.409 (8)	O3—Nd2^{viii}	2.601 (7)
Nd1—O2^{vii}	2.439 (7)	O3—Nd1^{ii}	2.641 (7)
Nd1—O7	2.455 (7)	O4—W2^{xii}	2.196 (7)
Nd1—O6	2.499 (7)	O4—Nd2^{iii}	2.743 (8)
Nd1—O7^{ii}	2.513 (7)	O5—Nd1^{vii}	2.377 (6)

Nd1—O8	2.618 (8)	O7—Nd2^{vi}	2.379 (6)
Nd1—O3^{ii}	2.641 (7)	O7—Nd1^{ii}	2.513 (7)
Nd1—O5^{iv}	3.096 (7)	O9—W1^{xiii}	1.990 (7)
Nd1—W1^{ii}	3.3885 (7)	O9—Nd1^{xi}	2.409 (8)

O2—W1—O8	100.9 (3)	O8—Nd1—Nd2^{vi}	84.50 (16)
O2—W1—O4	93.3 (3)	O3^{ii}—Nd1—Nd2^{vi}	43.46 (15)
O8—W1—O4	102.3 (3)	W1^{ii}—Nd1—Nd2^{vi}	81.091 (15)
O2—W1—O7	108.8 (3)	W1—Nd1—Nd2^{vi}	64.843 (14)
O8—W1—O7	84.6 (3)	O5^{vi}—Nd1—Nd2^{viii}	159.13 (18)
O4—W1—O7	155.3 (3)	O9^{iv}—Nd1—Nd2^{viii}	74.28 (17)
O2—W1—O9^{i}	94.2 (3)	O2^{vii}—Nd1—Nd2^{viii}	38.63 (18)
O8—W1—O9^{i}	160.6 (3)	O7—Nd1—Nd2^{viii}	84.99 (15)
O4—W1—O9^{i}	88.8 (3)	O6—Nd1—Nd2^{viii}	118.17 (17)
O7—W1—O9^{i}	79.0 (3)	O7^{ii}—Nd1—Nd2^{viii}	35.06 (14)
O2—W1—O3	166.6 (3)	O8—Nd1—Nd2^{viii}	86.62 (16)
O8—W1—O3	88.9 (3)	O3^{ii}—Nd1—Nd2^{viii}	98.06 (15)
O4—W1—O3	75.5 (3)	W1^{ii}—Nd1—Nd2^{viii}	64.182 (13)
O7—W1—O3	81.0 (3)	W1—Nd1—Nd2^{viii}	76.989 (16)
O9^{i}—W1—O3	78.4 (3)	Nd2^{vi}—Nd1—Nd2^{viii}	116.337 (18)
O2—W1—Nd1^{ii}	129.2 (2)	O8—Nd2—O7^{vii}	80.4 (2)
O8—W1—Nd1^{ii}	116.3 (2)	O8—Nd2—O1	149.9 (2)
O4—W1—Nd1^{ii}	110.0 (2)	O7^{vii}—Nd2—O1	129.0 (2)
O7—W1—Nd1^{ii}	47.2 (2)	O8—Nd2—O6	71.9 (3)
O9^{i}—W1—Nd1^{ii}	44.4 (2)	O7^{vii}—Nd2—O6	86.5 (2)
O3—W1—Nd1^{ii}	51.18 (18)	O1—Nd2—O6	111.1 (2)
O2—W1—Nd2^{iii}	45.4 (2)	O8—Nd2—O1^{ix}	79.9 (2)
O8—W1—Nd2^{iii}	122.5 (2)	O7^{vii}—Nd2—O1^{ix}	151.4 (2)
O4—W1—Nd2^{iii}	51.9 (2)	O1—Nd2—O1^{ix}	74.3 (3)
O7—W1—Nd2^{iii}	142.0 (2)	O6—Nd2—O1^{ix}	67.7 (2)
O9^{i}—W1—Nd2^{iii}	76.8 (2)	O8—Nd2—O2^{iii}	81.3 (3)
O3—W1—Nd2^{iii}	121.46 (17)	O7^{vii}—Nd2—O2^{iii}	74.0 (2)
Nd1^{ii}—W1—Nd2^{iii}	120.734 (19)	O1—Nd2—O2^{iii}	99.8 (2)
O2—W1—Nd1	123.3 (2)	O6—Nd2—O2^{iii}	149.1 (2)
O8—W1—Nd1	46.0 (2)	O1^{ix}—Nd2—O2^{iii}	122.9 (2)
O4—W1—Nd1	132.0 (2)	O8—Nd2—O5	128.2 (2)
O7—W1—Nd1	41.7 (2)	O7^{vii}—Nd2—O5	73.2 (2)
O9^{i}—W1—Nd1	115.0 (2)	O1—Nd2—O5	73.8 (2)
O3—W1—Nd1	70.08 (18)	O6—Nd2—O5	62.9 (2)
Nd1^{ii}—W1—Nd1	72.141 (17)	O1^{ix}—Nd2—O5	103.6 (2)
Nd2^{iii}—W1—Nd1	166.031 (17)	O2^{iii}—Nd2—O5	129.8 (2)
O1^{iv}—W2—O6	96.6 (3)	O8—Nd2—O3^{x}	139.7 (2)
O1^{iv}—W2—O5	106.8 (3)	O7^{vii}—Nd2—O3^{x}	66.3 (2)
O6—W2—O5	91.3 (3)	O1—Nd2—O3^{x}	64.6 (2)
O1^{iv}—W2—O3^{v}	93.3 (3)	O6—Nd2—O3^{x}	125.3 (2)
O6—W2—O3^{v}	98.6 (3)	O1^{ix}—Nd2—O3^{x}	138.9 (2)
O5—W2—O3^{v}	156.4 (3)	O2^{iii}—Nd2—O3^{x}	68.4 (2)
O1^{iv}—W2—O9	91.1 (3)	O5—Nd2—O3^{x}	64.0 (2)

O6—W2—O9	171.5 (3)
O5—W2—O9	83.0 (3)
O3^{v}—W2—O9	84.5 (3)
O1^{iv}—W2—O4^{v}	166.5 (3)
O6—W2—O4^{v}	90.9 (3)
O5—W2—O4^{v}	84.0 (3)
O3^{v}—W2—O4^{v}	74.5 (3)
O9—W2—O4^{v}	82.2 (3)
O1^{iv}—W2—Nd2^{iv}	44.5 (2)
O6—W2—Nd2^{iv}	109.4 (2)
O5—W2—Nd2^{iv}	144.8 (2)
O3^{v}—W2—Nd2^{iv}	50.0 (2)
O9—W2—Nd2^{iv}	78.7 (2)
O4^{v}—W2—Nd2^{iv}	122.34 (18)
O1^{iv}—W2—Nd2	120.5 (2)
O6—W2—Nd2	45.2 (2)
O5—W2—Nd2	49.4 (2)
O3^{v}—W2—Nd2	129.1 (2)
O9—W2—Nd2	127.1 (2)
O4^{v}—W2—Nd2	72.57 (19)
Nd2^{iv}—W2—Nd2	153.578 (17)
O5^{vi}—Nd1—O9^{iv}	108.0 (2)
O5^{vi}—Nd1—O2^{vii}	156.0 (2)
O9^{iv}—Nd1—O2^{vii}	92.4 (2)
O5^{vi}—Nd1—O7	75.9 (2)
O9^{iv}—Nd1—O7	119.6 (2)
O2^{vii}—Nd1—O7	105.4 (2)
O5^{vi}—Nd1—O6	79.4 (2)
O9^{iv}—Nd1—O6	119.7 (2)
O2^{vii}—Nd1—O6	79.5 (2)
O7—Nd1—O6	120.2 (2)
O5^{vi}—Nd1—O7^{ii}	127.1 (2)
O9^{iv}—Nd1—O7^{ii}	60.9 (2)
O2^{vii}—Nd1—O7^{ii}	73.7 (2)
O7—Nd1—O7^{ii}	69.7 (2)
O6—Nd1—O7^{ii}	153.1 (2)
O5^{vi}—Nd1—O8	90.9 (2)
O9^{iv}—Nd1—O8	160.7 (2)
O2^{vii}—Nd1—O8	70.3 (2)
O7—Nd1—O8	60.1 (2)
O6—Nd1—O8	66.9 (2)
O7^{ii}—Nd1—O8	104.5 (2)
O5^{vi}—Nd1—O3^{ii}	66.4 (2)
O9^{iv}—Nd1—O3^{ii}	63.2 (2)
O2^{vii}—Nd1—O3^{ii}	136.4 (2)
O7—Nd1—O3^{ii}	64.7 (2)
O6—Nd1—O3^{ii}	143.4 (2)
O7^{ii}—Nd1—O3^{ii}	63.0 (2)
O8—Nd2—O4^{iii}	91.3 (2)
O7^{vii}—Nd2—O4^{iii}	134.1 (2)
O1—Nd2—O4^{iii}	64.5 (2)
O6—Nd2—O4^{iii}	133.7 (2)
O1^{ix}—Nd2—O4^{iii}	67.0 (2)
O2^{iii}—Nd2—O4^{iii}	60.1 (2)
O5—Nd2—O4^{iii}	138.4 (2)
O3^{x}—Nd2—O4^{iii}	95.7 (2)
O8—Nd2—W2^{xi}	160.01 (19)
O7^{vii}—Nd2—W2^{xi}	100.57 (16)
O1—Nd2—W2^{xi}	30.95 (15)
O6—Nd2—W2^{xi}	128.07 (16)
O1^{ix}—Nd2—W2^{xi}	104.97 (16)
O2^{iii}—Nd2—W2^{xi}	79.85 (16)
O5—Nd2—W2^{xi}	70.14 (16)
O3^{x}—Nd2—W2^{xi}	34.37 (14)
O4^{iii}—Nd2—W2^{xi}	73.54 (16)
O8—Nd2—W2	103.17 (19)
O7^{vii}—Nd2—W2	86.45 (16)
O1—Nd2—W2	86.55 (17)
O6—Nd2—W2	31.75 (16)
O1^{ix}—Nd2—W2	77.98 (17)
O2^{iii}—Nd2—W2	159.08 (15)
O5—Nd2—W2	33.16 (14)
O3^{x}—Nd2—W2	97.17 (16)
O4^{iii}—Nd2—W2	139.03 (14)
W2^{xi}—Nd2—W2	96.814 (16)
O8—Nd2—W1^{iii}	93.93 (19)
O7^{vii}—Nd2—W1^{iii}	102.97 (16)
O1—Nd2—W1^{iii}	75.32 (17)
O6—Nd2—W1^{iii}	161.63 (17)
O1^{ix}—Nd2—W1^{iii}	98.99 (16)
O2^{iii}—Nd2—W1^{iii}	30.07 (15)
O5—Nd2—W1^{iii}	134.69 (15)
O3^{x}—Nd2—W1^{iii}	73.07 (16)
O4^{iii}—Nd2—W1^{iii}	32.17 (14)
W2^{xi}—Nd2—W1^{iii}	66.284 (15)
W2—Nd2—W1^{iii}	161.709 (19)
W2^{xi}—O1—Nd2	104.6 (3)
W2^{xi}—O1—Nd2^{ix}	148.7 (4)
Nd2—O1—Nd2^{ix}	105.7 (2)
W1—O2—Nd1^{vi}	145.5 (4)
W1—O2—Nd2^{iii}	104.6 (3)
Nd1^{vi}—O2—Nd2^{iii}	104.7 (3)
W2^{xii}—O3—W1	103.7 (3)
W2^{xii}—O3—Nd2^{viii}	95.7 (2)
W1—O3—Nd2^{viii}	152.7 (3)
W2^{xii}—O3—Nd1^{ii}	133.4 (3)

O8—Nd1—O3^{ii}	123.9 (2)
O5^{vi}—Nd1—W1^{ii}	105.15 (17)
O9^{iv}—Nd1—W1^{ii}	35.29 (17)
O2^{vii}—Nd1—W1^{ii}	98.77 (17)
O7—Nd1—W1^{ii}	84.57 (15)
O6—Nd1—W1^{ii}	154.94 (18)
O7^{ii}—Nd1—W1^{ii}	34.47 (14)
O8—Nd1—W1^{ii}	136.43 (15)
O3^{ii}—Nd1—W1^{ii}	40.51 (15)
O5^{vi}—Nd1—W1	90.51 (18)
O9^{iv}—Nd1—W1	141.30 (17)
O2^{vii}—Nd1—W1	80.66 (17)
O7—Nd1—W1	31.71 (14)
O6—Nd1—W1	96.60 (18)
O7^{ii}—Nd1—W1	80.69 (15)
O8—Nd1—W1	30.35 (15)
O3^{ii}—Nd1—W1	96.28 (15)
W1^{ii}—Nd1—W1	107.859 (18)
O5^{vi}—Nd1—Nd2^{vi}	42.80 (18)
O9^{iv}—Nd1—Nd2^{vi}	106.32 (16)
O2^{vii}—Nd1—Nd2^{vi}	143.23 (18)
O7—Nd1—Nd2^{vi}	37.87 (14)
O6—Nd1—Nd2^{vi}	115.25 (18)
O7^{ii}—Nd1—Nd2^{vi}	87.96 (15)
W1—O3—Nd1^{ii}	88.3 (2)
Nd2^{viii}—O3—Nd1^{ii}	92.2 (2)
W1—O4—W2^{xii}	106.1 (3)
W1—O4—Nd2^{iii}	95.9 (3)
W2^{xii}—O4—Nd2^{iii}	147.0 (3)
W2—O5—Nd1^{vii}	130.8 (4)
W2—O5—Nd2	97.5 (3)
Nd1^{vii}—O5—Nd2	98.8 (3)
W2—O6—Nd2	103.0 (3)
W2—O6—Nd1	145.6 (4)
Nd2—O6—Nd1	110.3 (3)
W1—O7—Nd2^{vi}	130.6 (3)
W1—O7—Nd1	106.5 (3)
Nd2^{vi}—O7—Nd1	102.8 (2)
W1—O7—Nd1^{ii}	98.3 (3)
Nd2^{vi}—O7—Nd1^{ii}	107.6 (2)
Nd1—O7—Nd1^{ii}	110.3 (2)
W1—O8—Nd2	143.0 (4)
W1—O8—Nd1	103.6 (3)
Nd2—O8—Nd1	110.9 (3)
W1^{xiii}—O9—W2	138.0 (4)
W1^{xiii}—O9—Nd1^{xi}	100.3 (3)
W2—O9—Nd1^{xi}	120.4 (3)

Symmetry codes: (i) x+1, $-y$+3/2, z−1/2; (ii) $-x$+1, $-y$+2, $-z$; (iii) $-x$+1, $-y$+1, $-z$; (iv) $-x$, y+1/2, $-z$+1/2; (v) x−1, y, z; (vi) x, $-y$+3/2, z−1/2; (vii) x, $-y$+3/2, z+1/2; (viii) $-x$+1, y+1/2, $-z$+1/2; (ix) $-x$, $-y$+1, $-z$; (x) $-x$+1, y−1/2, $-z$+1/2; (xi) $-x$, y−1/2, $-z$+1/2; (xii) x+1, y, z; (xiii) x−1, $-y$+3/2, z+1/2.