Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Tetrakis[$\mu$-2-(4-hydroxyphenyl)acetato]-$\kappa^3O,O':O;\kappa^3O:O,O'$-bis{aqua(4,4′-bipyridine-$\kappa N$)bis[2-(4-hydroxyphenyl)acetato-$\kappa^2O,O$]neodymium(III)} monohydrate

**Jia-Lu Liu, Jian-Feng Liu and Guo-Liang Zhao***

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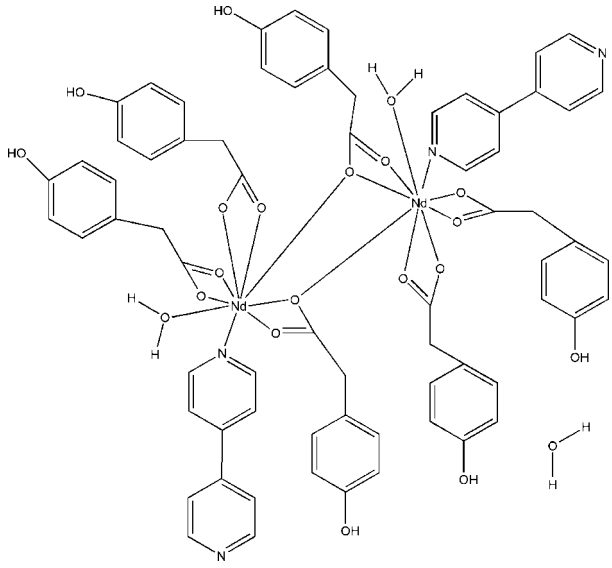
Received 9 October 2010; accepted 22 October 2010

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.021; $wR$ factor = 0.053; data-to-parameter ratio = 12.8.

The title complex, $[Nd_2(C_8H_7O_3)_6(C_{10}H_8N_2)_2(H_2O)_2]\cdot H_2O$, contains two Nd atoms, six 4-hydroxyphenylacetate (hpaa) anions, two 4,4′-bipyridine molecules (bipy) and two water molecules; an additional water molecule of solvation is also present in the crystal structure. Each of the $Nd^{III}$ ions is nine-coordinated by seven O atoms from four hpaa ligands, an N atom from a bipy ligand and an O atom from a water molecule in a distorted tricapped trigonal-prismatic geometry. The hpaa ligands are coordinated to the $Nd^{III}$ ions in the bridging and bridging tridentate modes. Extensive O—H···O, O—H···N and C—H···O hydrogen bonding stabilizes the crystal structure.

## Related literature

For related structures and background literature, see: Liu *et al.* (2010); Wang *et al.* (2010); Fang & Zhang (2006); Wang & Sevov (2008).



## Experimental

### Crystal data

$[Nd_2(C_8H_7O_3)_6(C_{10}H_8N_2)_2(H_2O)_2]\cdot H_2O$
$M_r$ = 1561.72
Triclinic, $P\overline{1}$
$a$ = 11.77540 (1) Å
$b$ = 16.3732 (2) Å
$c$ = 18.4864 (2) Å
$\alpha$ = 83.672 (1)°
$\beta$ = 71.926 (1)°
$\gamma$ = 70.814 (1)°
$V$ = 3199.99 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.69 mm$^{-1}$
$T$ = 296 K
0.25 × 0.24 × 0.07 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.668, $T_{max}$ = 0.883
41660 measured reflections
11220 independent reflections
9780 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.053
$S$ = 1.07
11220 reflections
875 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.51 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3$B$···O12$^{i}$ | 0.82 | 1.94 | 2.751 (3) | 170 |
| O6—H6$B$···O3$W^{ii}$ | 0.82 | 1.86 | 2.647 (3) | 160 |
| O9—H9$A$···O17$^{iii}$ | 0.82 | 1.86 | 2.676 (3) | 173 |
| O12—H12$A$···O11$^{iv}$ | 0.82 | 1.94 | 2.746 (2) | 167 |
| O15—H15$C$···O6$^{v}$ | 0.82 | 1.91 | 2.725 (3) | 173 |
| O18—H18$B$···O9$^{ii}$ | 0.82 | 1.95 | 2.763 (3) | 173 |
| O2$W$—H2$WA$···O5 | 0.82 (2) | 2.02 (2) | 2.772 (2) | 153 (3) |
| O2$W$—H2$WB$···N2$^{ii}$ | 0.81 (2) | 2.04 (2) | 2.840 (3) | 170 (3) |
| O3$W$—H3$WB$···O3 | 0.82 (2) | 2.02 (2) | 2.811 (3) | 162 (3) |
| O1$W$—H1$WA$···O13 | 0.81 (2) | 1.98 (2) | 2.764 (2) | 161 (3) |
| O1$W$—H1$WB$···N4$^{i}$ | 0.82 (2) | 1.99 (2) | 2.775 (3) | 161 (3) |
| O3$W$—H3$WA$···O1$^{vi}$ | 0.82 (2) | 1.95 (2) | 2.770 (3) | 175 (4) |
| C6—H6$A$···O2$^{vii}$ | 0.93 | 2.49 | 3.283 (3) | 144 |

Symmetry codes: (i) $x, y+1, z$; (ii) $x, y-1, z$; (iii) $-x, -y+1, -z$; (iv) $-x, -y, -z+1$; (v) $x-1, y+1, z$; (vi) $-x+1, -y+1, -z+1$; (vii) $-x, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

**Any acknowledgements?**

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2337).

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# supporting information

*Acta Cryst.* (2010). E**66**, m1476–m1477 [https://doi.org/10.1107/S1600536810043023]

# Tetrakis[$\mu$-2-(4-hydroxyphenyl)acetato]-$\kappa^3O,O':O;\kappa^3O:O,O'$-bis{aqua(4,4′-bipyridine-$\kappa N$)bis[2-(4-hydroxyphenyl)acetato-$\kappa^2O,O$]neodymium(III)} monohydrate

**Jia-Lu Liu, Jian-Feng Liu and Guo-Liang Zhao**

## S1. Comment

There has been an increasing interest in the design and synthesis of carboxylic metal-organic complexes owing to their potential practical applications, such as fluorescence, magnetism, etc. (Wang, *et al.*, 2010; Fang & Zhang, 2006; Wang & Sevov, 2008). In continuation to our research (Liu, *et al.*, 2010), we now report the preparation and crystal structure of a new neodymium$^{III}$ complex with the ligand 4-hydroxyphenylacetic acid (hpaa).

The crystal structure of the title complex (Fig. 1) contains two Nd atoms, six (hpaa) molecules, two 4,4′-bipyridine molecules (bipy) and two water molecules; an additional water molecule of solvation is also present which is not involved in coordination. Each Nd atom is nine coordinated. The (hpaa) ligands are coordinated by two modes, bridging and bridging tridentate. The neodymium$^{III}$ atom is in a distort capped pentagonal prism environment. The Nd—O bond lengths range from 2.4180 (15) to 2.6237 (16) Å. The Nd—N distances range from 2.6325 (19) to 2.6544 (18) Å. The Nd—O(water) bond lengths ranging from 2.4816 (16) to 2.4847 (16) Å, are slightly shorter than the other Nd—O bond distances. In addition, there are several hydrogen bonds in the crystal structure which strengthen the stability of the crystal structure (Table 1).

## S2. Experimental

A solution of 4-hydroxyphenylacetic acid (hpaa) (30 ml) in distilled water (20 ml) was mixed with a solution of sodium hydroxide (30 mmol) in distilled water (20 ml) and the solution and diluted to 100 ml. To a 10 ml portion of this sodium salt solution a solution of $Nd(NO_3)_3$ (1 mmol) in distilled water (10 ml) was added in a dropwise fashion. After about an hour, 4,4′-bipyridine (1 mmol) in ethanol (5 ml) was slowly dripped into the solution, stirred for three hours and filtered. After allowing the filtrate to stand for a week, a mass of colorless crystals was obtained.

## S3. Refinement

The H-atoms of the water molecules were located from differencne maps and were included in the subsequent refinement using the restraints (O—H = 0.82 (1)Å, H···H = 1.39 (2)Å) with $U_{iso}$(H) = 1.5$U_{eq}$(O). The remaining H atoms were positioned geometrically and refined using a riding model with O—H = 0.82 Å and C—H = 0.93 and 0.97 Å for aryl and methylene type H-atoms, respectively with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(O).

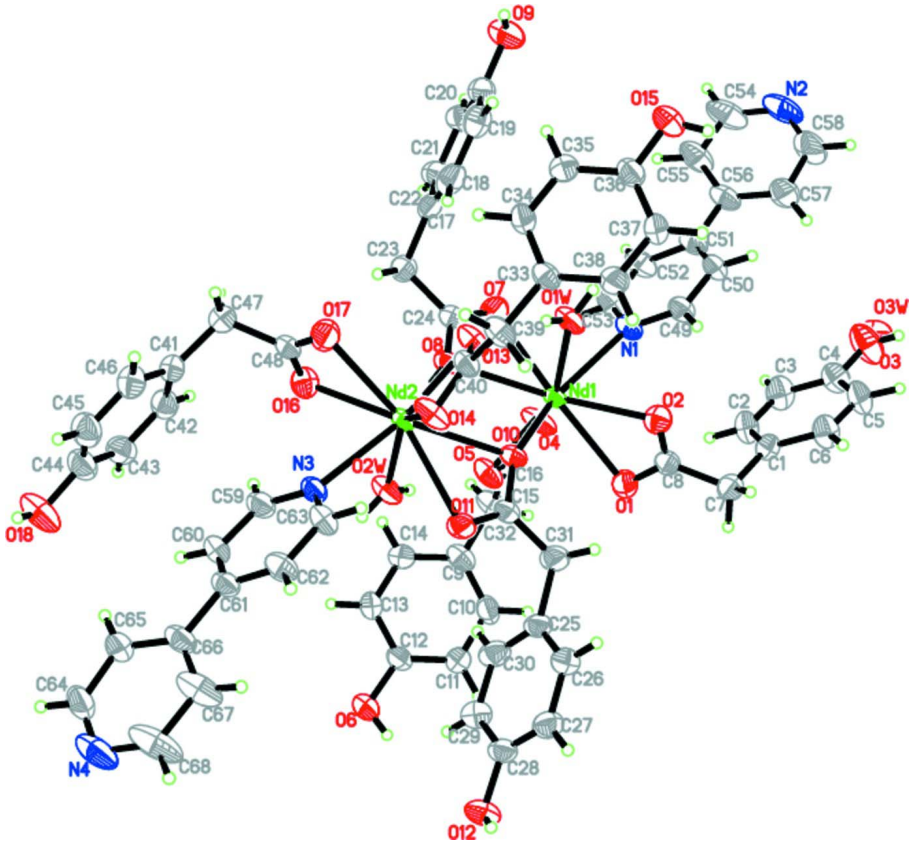


**Figure 1**

The molecular structure of the title complex, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

**Tetrakis[$\mu$-2-(4-hydroxyphenyl)acetato]- $\kappa^3O,O':O;\kappa^3O:O,O'$- bis{aqua(4,4′-bipyridine-$\kappa N$)bis[2-(4-hydroxyphenyl)acetato- $\kappa^2O,O$]neodymium(III)} monohydrate**

*Crystal data*

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$\gamma$ = 70.814 (1)°
$V$ = 3199.99 (6) Å$^3$
$Z$ = 2
$F(000)$ = 1576
$D_x$ = 1.621 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9932 reflections
$\theta$ = 1.7–25.0°
$\mu$ = 1.69 mm$^{-1}$
$T$ = 296 K
Block, colourless
0.25 × 0.24 × 0.07 mm

*Data collection*

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
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41660 measured reflections
11220 independent reflections

9780 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -14 \rightarrow 14$
$k = -19 \rightarrow 19$
$l = -21 \rightarrow 21$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.053$
$S = 1.07$
11220 reflections
875 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 0.9476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.37$ e Å$^{-3}$
$\Delta\rho_{min} = -0.51$ e Å$^{-3}$

*Special details*

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

**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 $F^2 > \sigma(F^2)$ 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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Nd1 | 0.270706 (11) | 0.364834 (7) | 0.284566 (7) | 0.02466 (4) |
| Nd2 | 0.132489 (11) | 0.205750 (7) | 0.194233 (7) | 0.02465 (4) |
| N1 | 0.3145 (2) | 0.51275 (12) | 0.28312 (12) | 0.0344 (5) |
| N2 | 0.3992 (3) | 0.92555 (16) | 0.2132 (2) | 0.0641 (8) |
| N3 | 0.08245 (19) | 0.06055 (12) | 0.18750 (11) | 0.0321 (5) |
| N4 | 0.0249 (3) | −0.36120 (16) | 0.2350 (2) | 0.0665 (8) |
| C1 | 0.2239 (2) | 0.51251 (16) | 0.51879 (13) | 0.0336 (6) |
| C2 | 0.3397 (3) | 0.51654 (18) | 0.47391 (15) | 0.0447 (7) |
| H2A | 0.3955 | 0.4690 | 0.4448 | 0.054* |
| C3 | 0.3749 (3) | 0.58985 (19) | 0.47123 (16) | 0.0498 (7) |
| H3A | 0.4529 | 0.5917 | 0.4399 | 0.060* |
| C4 | 0.2944 (3) | 0.65967 (17) | 0.51496 (16) | 0.0431 (7) |
| C5 | 0.1802 (3) | 0.65599 (18) | 0.56189 (16) | 0.0467 (7) |
| H5A | 0.1267 | 0.7025 | 0.5930 | 0.056* |
| C6 | 0.1446 (3) | 0.58383 (17) | 0.56302 (15) | 0.0434 (7) |
| H6A | 0.0659 | 0.5828 | 0.5940 | 0.052* |
| C7 | 0.1849 (3) | 0.43233 (17) | 0.52304 (14) | 0.0400 (6) |
| H7A | 0.2317 | 0.3874 | 0.5511 | 0.048* |
| H7B | 0.0963 | 0.4455 | 0.5504 | 0.048* |
| C8 | 0.2082 (2) | 0.39955 (16) | 0.44499 (14) | 0.0339 (6) |
| C9 | 0.6231 (2) | 0.08712 (16) | 0.30460 (15) | 0.0368 (6) |

| | | | | |
|---|---|---|---|---|
| C10 | 0.6052 (3) | 0.05562 (17) | 0.37775 (16) | 0.0461 (7) |
| H10A | 0.5935 | 0.0919 | 0.4165 | 0.055* |
| C11 | 0.6039 (3) | −0.02832 (17) | 0.39577 (15) | 0.0466 (7) |
| H11A | 0.5932 | −0.0482 | 0.4458 | 0.056* |
| C12 | 0.6186 (2) | −0.08206 (15) | 0.33954 (14) | 0.0369 (6) |
| C13 | 0.6359 (3) | −0.05165 (17) | 0.26549 (14) | 0.0422 (7) |
| H13A | 0.6463 | −0.0879 | 0.2270 | 0.051* |
| C14 | 0.6378 (3) | 0.03113 (16) | 0.24858 (15) | 0.0408 (6) |
| H14A | 0.6493 | 0.0506 | 0.1984 | 0.049* |
| C15 | 0.6270 (3) | 0.17779 (16) | 0.28492 (18) | 0.0471 (7) |
| H15A | 0.6946 | 0.1763 | 0.2384 | 0.057* |
| H15B | 0.6472 | 0.1986 | 0.3250 | 0.057* |
| C16 | 0.5074 (2) | 0.24161 (15) | 0.27414 (14) | 0.0330 (6) |
| C17 | 0.2717 (3) | 0.45494 (17) | 0.01296 (14) | 0.0415 (7) |
| C18 | 0.1461 (3) | 0.50163 (19) | 0.02788 (14) | 0.0482 (7) |
| H18A | 0.0863 | 0.4747 | 0.0534 | 0.058* |
| C19 | 0.1064 (3) | 0.58758 (19) | 0.00594 (15) | 0.0450 (7) |
| H19A | 0.0210 | 0.6179 | 0.0170 | 0.054* |
| C20 | 0.1948 (3) | 0.62755 (17) | −0.03244 (14) | 0.0387 (6) |
| C21 | 0.3209 (3) | 0.58215 (17) | −0.04733 (15) | 0.0419 (6) |
| H21A | 0.3809 | 0.6091 | −0.0724 | 0.050* |
| C22 | 0.3581 (3) | 0.49691 (17) | −0.02502 (15) | 0.0425 (7) |
| H22A | 0.4434 | 0.4668 | −0.0358 | 0.051* |
| C23 | 0.3127 (3) | 0.36227 (18) | 0.03879 (15) | 0.0576 (9) |
| H23A | 0.3977 | 0.3338 | 0.0079 | 0.069* |
| H23B | 0.2583 | 0.3328 | 0.0310 | 0.069* |
| C24 | 0.3091 (2) | 0.35461 (15) | 0.12153 (13) | 0.0327 (6) |
| C25 | 0.1422 (3) | 0.11229 (16) | 0.47574 (14) | 0.0380 (6) |
| C26 | 0.0397 (3) | 0.10565 (17) | 0.53565 (14) | 0.0422 (6) |
| H26A | −0.0291 | 0.1547 | 0.5516 | 0.051* |
| C27 | 0.0379 (3) | 0.02725 (17) | 0.57209 (14) | 0.0413 (6) |
| H27A | −0.0311 | 0.0239 | 0.6125 | 0.050* |
| C28 | 0.1390 (2) | −0.04569 (16) | 0.54792 (14) | 0.0349 (6) |
| C29 | 0.2418 (3) | −0.04044 (18) | 0.48871 (15) | 0.0414 (6) |
| H29A | 0.3102 | −0.0896 | 0.4724 | 0.050* |
| C30 | 0.2424 (3) | 0.03838 (18) | 0.45375 (15) | 0.0419 (6) |
| H30A | 0.3125 | 0.0417 | 0.4142 | 0.050* |
| C31 | 0.1436 (3) | 0.19656 (17) | 0.43415 (14) | 0.0458 (7) |
| H31A | 0.2246 | 0.2043 | 0.4272 | 0.055* |
| H31B | 0.0800 | 0.2434 | 0.4658 | 0.055* |
| C32 | 0.1205 (2) | 0.20377 (15) | 0.35757 (13) | 0.0291 (5) |
| C33 | −0.2574 (2) | 0.48110 (15) | 0.24444 (14) | 0.0308 (5) |
| C34 | −0.2146 (2) | 0.51905 (16) | 0.17483 (14) | 0.0369 (6) |
| H34A | −0.1765 | 0.4848 | 0.1316 | 0.044* |
| C35 | −0.2266 (3) | 0.60524 (16) | 0.16765 (14) | 0.0400 (6) |
| H35A | −0.1973 | 0.6287 | 0.1200 | 0.048* |
| C36 | −0.2821 (2) | 0.65779 (16) | 0.23092 (14) | 0.0367 (6) |
| C37 | −0.3248 (3) | 0.62160 (16) | 0.30103 (14) | 0.0400 (6) |

| | | | | |
|---|---|---|---|---|
| H37A | −0.3622 | 0.6560 | 0.3441 | 0.048* |
| C38 | −0.3121 (2) | 0.53431 (16) | 0.30741 (14) | 0.0373 (6) |
| H38A | −0.3408 | 0.5108 | 0.3551 | 0.045* |
| C39 | −0.2452 (2) | 0.38659 (15) | 0.25102 (15) | 0.0375 (6) |
| H39A | −0.2904 | 0.3748 | 0.3026 | 0.045* |
| H39B | −0.2863 | 0.3744 | 0.2172 | 0.045* |
| C40 | −0.1139 (2) | 0.32540 (15) | 0.23301 (13) | 0.0303 (5) |
| C41 | 0.2356 (3) | 0.05071 (16) | −0.04968 (13) | 0.0381 (6) |
| C42 | 0.3543 (3) | −0.00084 (17) | −0.04648 (14) | 0.0401 (6) |
| H42A | 0.4115 | 0.0256 | −0.0433 | 0.048* |
| C43 | 0.3896 (3) | −0.08951 (17) | −0.04784 (14) | 0.0433 (6) |
| H43A | 0.4698 | −0.1224 | −0.0460 | 0.052* |
| C44 | 0.3055 (3) | −0.12956 (18) | −0.05194 (16) | 0.0470 (7) |
| C45 | 0.1880 (3) | −0.08015 (19) | −0.05647 (16) | 0.0493 (7) |
| H45A | 0.1317 | −0.1069 | −0.0603 | 0.059* |
| C46 | 0.1535 (3) | 0.00887 (18) | −0.05533 (14) | 0.0438 (7) |
| H46A | 0.0739 | 0.0415 | −0.0584 | 0.053* |
| C47 | 0.1944 (3) | 0.14797 (17) | −0.04442 (14) | 0.0449 (7) |
| H47A | 0.1165 | 0.1723 | −0.0578 | 0.054* |
| H47B | 0.2576 | 0.1696 | −0.0808 | 0.054* |
| C48 | 0.1751 (3) | 0.17737 (15) | 0.03463 (14) | 0.0350 (6) |
| C49 | 0.2327 (2) | 0.58181 (15) | 0.32258 (14) | 0.0364 (6) |
| H49A | 0.1603 | 0.5758 | 0.3583 | 0.044* |
| C50 | 0.2504 (3) | 0.66216 (15) | 0.31305 (14) | 0.0381 (6) |
| H50A | 0.1908 | 0.7087 | 0.3420 | 0.046* |
| C51 | 0.3571 (2) | 0.67304 (15) | 0.26029 (15) | 0.0356 (6) |
| C52 | 0.4435 (2) | 0.60051 (16) | 0.22073 (16) | 0.0430 (7) |
| H52A | 0.5176 | 0.6043 | 0.1854 | 0.052* |
| C53 | 0.4191 (3) | 0.52275 (16) | 0.23395 (16) | 0.0415 (6) |
| H53A | 0.4786 | 0.4747 | 0.2072 | 0.050* |
| C54 | 0.4499 (3) | 0.8642 (2) | 0.1607 (2) | 0.0668 (10) |
| H54A | 0.4940 | 0.8778 | 0.1122 | 0.080* |
| C55 | 0.4411 (3) | 0.78141 (18) | 0.17384 (19) | 0.0564 (8) |
| H55A | 0.4787 | 0.7410 | 0.1350 | 0.068* |
| C56 | 0.3761 (3) | 0.75937 (16) | 0.24497 (17) | 0.0420 (7) |
| C57 | 0.3254 (3) | 0.82212 (18) | 0.30020 (18) | 0.0592 (9) |
| H57A | 0.2826 | 0.8101 | 0.3495 | 0.071* |
| C58 | 0.3392 (4) | 0.9033 (2) | 0.2810 (2) | 0.0715 (10) |
| H58A | 0.3035 | 0.9449 | 0.3189 | 0.086* |
| C59 | 0.1674 (3) | −0.00571 (16) | 0.14551 (14) | 0.0382 (6) |
| H59A | 0.2399 | 0.0029 | 0.1120 | 0.046* |
| C60 | 0.1531 (3) | −0.08665 (16) | 0.14932 (15) | 0.0407 (6) |
| H60A | 0.2148 | −0.1305 | 0.1181 | 0.049* |
| C61 | 0.0480 (2) | −0.10279 (15) | 0.19916 (14) | 0.0351 (6) |
| C62 | −0.0423 (2) | −0.03258 (16) | 0.24109 (15) | 0.0396 (6) |
| H62A | −0.1164 | −0.0391 | 0.2744 | 0.047* |
| C63 | −0.0223 (2) | 0.04660 (16) | 0.23338 (15) | 0.0370 (6) |
| H63A | −0.0848 | 0.0927 | 0.2615 | 0.044* |

| | | | | |
|---|---|---|---|---|
| C64 | 0.1031 (4) | −0.33921 (19) | 0.1736 (2) | 0.0719 (11) |
| H64A | 0.1558 | −0.3822 | 0.1385 | 0.086* |
| C65 | 0.1115 (4) | −0.25666 (18) | 0.15800 (17) | 0.0617 (9) |
| H65A | 0.1674 | −0.2451 | 0.1132 | 0.074* |
| C66 | 0.0362 (3) | −0.19106 (16) | 0.20950 (16) | 0.0417 (7) |
| C67 | −0.0466 (3) | −0.21345 (19) | 0.2739 (2) | 0.0596 (9) |
| H67A | −0.0998 | −0.1721 | 0.3104 | 0.072* |
| C68 | −0.0495 (3) | −0.2978 (2) | 0.2833 (3) | 0.0740 (11) |
| H68A | −0.1074 | −0.3109 | 0.3263 | 0.089* |
| O1W | 0.07774 (17) | 0.46117 (11) | 0.25536 (11) | 0.0393 (4) |
| H1WA | 0.034 (2) | 0.4394 (16) | 0.2422 (16) | 0.059* |
| H1WB | 0.045 (3) | 0.5134 (10) | 0.2533 (17) | 0.059* |
| O1 | 0.30329 (18) | 0.33594 (11) | 0.41748 (10) | 0.0445 (5) |
| O2W | 0.33238 (17) | 0.10872 (11) | 0.21403 (12) | 0.0406 (4) |
| H2WA | 0.379 (2) | 0.1269 (16) | 0.2276 (17) | 0.061* |
| H2WB | 0.360 (3) | 0.0565 (11) | 0.2138 (17) | 0.061* |
| O2 | 0.13434 (16) | 0.43730 (11) | 0.40659 (9) | 0.0384 (4) |
| O3 | 0.3315 (2) | 0.73205 (14) | 0.51087 (13) | 0.0660 (6) |
| H3B | 0.2736 | 0.7706 | 0.5367 | 0.057 (10)* |
| O3W | 0.5579 (2) | 0.76681 (14) | 0.49067 (13) | 0.0566 (5) |
| H3WA | 0.603 (3) | 0.736 (2) | 0.5157 (18) | 0.085* |
| H3WB | 0.502 (2) | 0.746 (2) | 0.495 (2) | 0.085* |
| O4 | 0.49884 (16) | 0.32022 (11) | 0.26571 (11) | 0.0469 (5) |
| O5 | 0.41618 (16) | 0.21614 (10) | 0.27630 (10) | 0.0398 (4) |
| O6 | 0.6197 (2) | −0.16628 (11) | 0.35255 (11) | 0.0572 (6) |
| H6B | 0.5929 | −0.1745 | 0.3984 | 0.086* |
| O7 | 0.35297 (18) | 0.40041 (12) | 0.14693 (10) | 0.0463 (5) |
| O8 | 0.25908 (15) | 0.30193 (10) | 0.16424 (9) | 0.0306 (4) |
| O9 | 0.16217 (19) | 0.71234 (12) | −0.05605 (12) | 0.0557 (5) |
| H9A | 0.0916 | 0.7266 | −0.0613 | 0.084* |
| O10 | 0.14216 (15) | 0.26635 (10) | 0.31474 (9) | 0.0294 (4) |
| O11 | 0.08199 (16) | 0.15084 (10) | 0.33586 (9) | 0.0370 (4) |
| O12 | 0.14175 (18) | −0.12543 (11) | 0.58121 (10) | 0.0462 (5) |
| H12A | 0.0698 | −0.1254 | 0.6038 | 0.069* |
| O13 | −0.01952 (15) | 0.35251 (10) | 0.20624 (10) | 0.0381 (4) |
| O14 | −0.09706 (16) | 0.24565 (10) | 0.24352 (11) | 0.0426 (4) |
| O15 | −0.2924 (2) | 0.74313 (11) | 0.22082 (11) | 0.0532 (5) |
| H15C | −0.3189 | 0.7666 | 0.2624 | 0.080* |
| O16 | 0.26326 (17) | 0.15156 (11) | 0.06384 (10) | 0.0407 (4) |
| O17 | 0.06975 (18) | 0.22670 (12) | 0.07132 (10) | 0.0480 (5) |
| O18 | 0.3439 (2) | −0.21795 (13) | −0.05134 (14) | 0.0743 (7) |
| H18B | 0.2876 | −0.2349 | −0.0548 | 0.111* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Nd1 | 0.02896 (8) | 0.01707 (7) | 0.03149 (7) | −0.00971 (5) | −0.01188 (6) | 0.00237 (5) |
| Nd2 | 0.02733 (8) | 0.01603 (7) | 0.03255 (8) | −0.00763 (5) | −0.01066 (6) | 0.00014 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1 | 0.0364 (13) | 0.0231 (11) | 0.0473 (13) | −0.0117 (10) | −0.0151 (10) | 0.0010 (9) |
| N2 | 0.0659 (19) | 0.0310 (14) | 0.113 (2) | −0.0255 (14) | −0.0456 (18) | 0.0175 (16) |
| N3 | 0.0381 (13) | 0.0221 (10) | 0.0388 (12) | −0.0111 (9) | −0.0133 (10) | 0.0000 (9) |
| N4 | 0.084 (2) | 0.0321 (15) | 0.115 (3) | −0.0280 (15) | −0.069 (2) | 0.0194 (16) |
| C1 | 0.0357 (15) | 0.0368 (14) | 0.0301 (13) | −0.0119 (12) | −0.0107 (11) | −0.0017 (11) |
| C2 | 0.0404 (17) | 0.0411 (16) | 0.0478 (16) | −0.0082 (13) | −0.0062 (13) | −0.0148 (13) |
| C3 | 0.0367 (16) | 0.0538 (18) | 0.0545 (18) | −0.0175 (14) | −0.0003 (14) | −0.0099 (14) |
| C4 | 0.0382 (16) | 0.0398 (16) | 0.0551 (17) | −0.0167 (13) | −0.0131 (14) | −0.0027 (13) |
| C5 | 0.0406 (17) | 0.0355 (15) | 0.0563 (18) | −0.0074 (13) | −0.0033 (14) | −0.0150 (13) |
| C6 | 0.0336 (15) | 0.0449 (16) | 0.0494 (16) | −0.0149 (13) | −0.0026 (13) | −0.0106 (13) |
| C7 | 0.0505 (17) | 0.0384 (15) | 0.0335 (14) | −0.0184 (13) | −0.0109 (12) | 0.0001 (11) |
| C8 | 0.0436 (16) | 0.0290 (14) | 0.0335 (13) | −0.0201 (13) | −0.0088 (12) | 0.0022 (11) |
| C9 | 0.0255 (14) | 0.0283 (13) | 0.0579 (17) | −0.0037 (11) | −0.0188 (12) | −0.0004 (12) |
| C10 | 0.0608 (19) | 0.0304 (15) | 0.0484 (17) | −0.0046 (13) | −0.0250 (15) | −0.0096 (12) |
| C11 | 0.066 (2) | 0.0367 (16) | 0.0339 (14) | −0.0104 (14) | −0.0165 (14) | −0.0007 (12) |
| C12 | 0.0429 (16) | 0.0258 (13) | 0.0423 (15) | −0.0101 (12) | −0.0140 (12) | 0.0015 (11) |
| C13 | 0.0577 (19) | 0.0342 (15) | 0.0361 (14) | −0.0133 (13) | −0.0146 (13) | −0.0068 (11) |
| C14 | 0.0483 (17) | 0.0340 (15) | 0.0379 (15) | −0.0109 (13) | −0.0131 (13) | 0.0040 (12) |
| C15 | 0.0371 (16) | 0.0281 (14) | 0.082 (2) | −0.0089 (12) | −0.0286 (15) | 0.0059 (14) |
| C16 | 0.0327 (14) | 0.0267 (13) | 0.0400 (14) | −0.0078 (11) | −0.0122 (11) | −0.0021 (11) |
| C17 | 0.069 (2) | 0.0403 (15) | 0.0274 (13) | −0.0289 (15) | −0.0194 (13) | 0.0045 (11) |
| C18 | 0.068 (2) | 0.060 (2) | 0.0315 (14) | −0.0443 (18) | −0.0107 (14) | 0.0042 (13) |
| C19 | 0.0449 (17) | 0.0550 (18) | 0.0403 (15) | −0.0203 (15) | −0.0125 (13) | −0.0073 (13) |
| C20 | 0.0484 (17) | 0.0359 (15) | 0.0420 (15) | −0.0182 (13) | −0.0231 (13) | 0.0027 (12) |
| C21 | 0.0488 (18) | 0.0377 (15) | 0.0485 (16) | −0.0251 (14) | −0.0182 (13) | 0.0097 (12) |
| C22 | 0.0488 (17) | 0.0375 (15) | 0.0472 (16) | −0.0164 (14) | −0.0210 (14) | 0.0058 (12) |
| C23 | 0.111 (3) | 0.0376 (16) | 0.0385 (16) | −0.0399 (18) | −0.0268 (17) | 0.0067 (13) |
| C24 | 0.0428 (15) | 0.0255 (13) | 0.0308 (13) | −0.0129 (12) | −0.0104 (12) | 0.0024 (10) |
| C25 | 0.0587 (18) | 0.0351 (15) | 0.0343 (14) | −0.0269 (14) | −0.0236 (13) | 0.0098 (11) |
| C26 | 0.0539 (18) | 0.0334 (14) | 0.0403 (15) | −0.0115 (13) | −0.0182 (14) | 0.0026 (12) |
| C27 | 0.0473 (17) | 0.0431 (16) | 0.0347 (14) | −0.0202 (14) | −0.0093 (13) | 0.0060 (12) |
| C28 | 0.0434 (16) | 0.0323 (14) | 0.0364 (14) | −0.0189 (13) | −0.0170 (12) | 0.0080 (11) |
| C29 | 0.0411 (16) | 0.0428 (16) | 0.0416 (15) | −0.0149 (13) | −0.0138 (13) | 0.0053 (12) |
| C30 | 0.0469 (17) | 0.0485 (17) | 0.0367 (15) | −0.0269 (15) | −0.0117 (13) | 0.0101 (12) |
| C31 | 0.075 (2) | 0.0388 (16) | 0.0403 (15) | −0.0341 (15) | −0.0263 (15) | 0.0096 (12) |
| C32 | 0.0314 (14) | 0.0226 (12) | 0.0337 (13) | −0.0107 (11) | −0.0085 (11) | 0.0025 (10) |
| C33 | 0.0236 (13) | 0.0245 (12) | 0.0432 (14) | −0.0033 (10) | −0.0118 (11) | −0.0026 (11) |
| C34 | 0.0395 (15) | 0.0308 (14) | 0.0366 (14) | −0.0051 (12) | −0.0091 (12) | −0.0086 (11) |
| C35 | 0.0500 (17) | 0.0358 (15) | 0.0316 (14) | −0.0139 (13) | −0.0089 (12) | 0.0027 (11) |
| C36 | 0.0415 (16) | 0.0270 (13) | 0.0443 (15) | −0.0098 (12) | −0.0169 (13) | −0.0017 (11) |
| C37 | 0.0493 (17) | 0.0309 (14) | 0.0358 (14) | −0.0048 (13) | −0.0122 (13) | −0.0091 (11) |
| C38 | 0.0384 (15) | 0.0326 (14) | 0.0348 (14) | −0.0063 (12) | −0.0080 (12) | 0.0010 (11) |
| C39 | 0.0292 (14) | 0.0273 (13) | 0.0533 (16) | −0.0059 (11) | −0.0107 (12) | −0.0024 (12) |
| C40 | 0.0320 (14) | 0.0223 (13) | 0.0393 (14) | −0.0078 (11) | −0.0141 (11) | −0.0027 (10) |
| C41 | 0.0501 (17) | 0.0341 (14) | 0.0290 (13) | −0.0130 (13) | −0.0092 (12) | −0.0036 (11) |
| C42 | 0.0450 (17) | 0.0414 (16) | 0.0382 (15) | −0.0220 (14) | −0.0086 (12) | −0.0016 (12) |
| C43 | 0.0438 (17) | 0.0376 (16) | 0.0446 (16) | −0.0101 (13) | −0.0108 (13) | 0.0013 (12) |
| C44 | 0.056 (2) | 0.0351 (16) | 0.0508 (17) | −0.0201 (14) | −0.0102 (14) | −0.0015 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C45 | 0.055 (2) | 0.0476 (18) | 0.0532 (18) | −0.0263 (16) | −0.0138 (15) | −0.0044 (14) |
| C46 | 0.0430 (17) | 0.0467 (17) | 0.0403 (15) | −0.0116 (14) | −0.0102 (13) | −0.0076 (12) |
| C47 | 0.0617 (19) | 0.0361 (15) | 0.0345 (14) | −0.0120 (14) | −0.0143 (14) | 0.0001 (12) |
| C48 | 0.0498 (17) | 0.0210 (13) | 0.0355 (14) | −0.0146 (12) | −0.0114 (13) | 0.0019 (11) |
| C49 | 0.0390 (15) | 0.0280 (14) | 0.0419 (15) | −0.0118 (12) | −0.0104 (12) | 0.0011 (11) |
| C50 | 0.0468 (17) | 0.0218 (13) | 0.0450 (15) | −0.0084 (12) | −0.0142 (13) | −0.0029 (11) |
| C51 | 0.0394 (15) | 0.0223 (13) | 0.0528 (16) | −0.0132 (12) | −0.0222 (13) | 0.0057 (11) |
| C52 | 0.0292 (15) | 0.0298 (14) | 0.0679 (19) | −0.0121 (12) | −0.0095 (13) | 0.0031 (13) |
| C53 | 0.0362 (16) | 0.0236 (13) | 0.0624 (18) | −0.0101 (12) | −0.0089 (14) | −0.0048 (12) |
| C54 | 0.052 (2) | 0.0389 (19) | 0.104 (3) | −0.0221 (16) | −0.0156 (19) | 0.0216 (19) |
| C55 | 0.0459 (18) | 0.0321 (16) | 0.082 (2) | −0.0153 (14) | −0.0042 (16) | 0.0023 (15) |
| C56 | 0.0418 (16) | 0.0254 (14) | 0.0667 (19) | −0.0128 (12) | −0.0265 (15) | 0.0052 (13) |
| C57 | 0.093 (3) | 0.0367 (17) | 0.062 (2) | −0.0328 (17) | −0.0308 (19) | 0.0038 (14) |
| C58 | 0.108 (3) | 0.0358 (18) | 0.093 (3) | −0.032 (2) | −0.049 (2) | −0.0025 (18) |
| C59 | 0.0447 (16) | 0.0278 (14) | 0.0405 (15) | −0.0140 (12) | −0.0083 (13) | 0.0024 (11) |
| C60 | 0.0547 (18) | 0.0236 (13) | 0.0418 (15) | −0.0085 (13) | −0.0142 (13) | −0.0035 (11) |
| C61 | 0.0463 (16) | 0.0247 (13) | 0.0460 (15) | −0.0146 (12) | −0.0280 (13) | 0.0060 (11) |
| C62 | 0.0365 (15) | 0.0310 (14) | 0.0545 (17) | −0.0160 (12) | −0.0136 (13) | 0.0039 (12) |
| C63 | 0.0364 (15) | 0.0247 (13) | 0.0501 (16) | −0.0091 (12) | −0.0118 (13) | −0.0048 (11) |
| C64 | 0.136 (4) | 0.0330 (17) | 0.073 (2) | −0.028 (2) | −0.066 (3) | 0.0020 (16) |
| C65 | 0.116 (3) | 0.0343 (17) | 0.0529 (18) | −0.0323 (18) | −0.0421 (19) | 0.0052 (14) |
| C66 | 0.0543 (18) | 0.0262 (14) | 0.0615 (18) | −0.0180 (13) | −0.0373 (15) | 0.0084 (13) |
| C67 | 0.0435 (18) | 0.0326 (16) | 0.103 (3) | −0.0135 (14) | −0.0239 (18) | 0.0126 (16) |
| C68 | 0.050 (2) | 0.0388 (19) | 0.141 (4) | −0.0242 (17) | −0.038 (2) | 0.027 (2) |
| O1W | 0.0440 (12) | 0.0192 (9) | 0.0619 (12) | −0.0072 (8) | −0.0286 (10) | 0.0002 (9) |
| O1 | 0.0541 (13) | 0.0363 (11) | 0.0409 (10) | −0.0022 (9) | −0.0219 (9) | −0.0056 (8) |
| O2W | 0.0381 (11) | 0.0217 (9) | 0.0681 (13) | −0.0072 (8) | −0.0264 (9) | 0.0000 (9) |
| O2 | 0.0369 (10) | 0.0406 (10) | 0.0386 (10) | −0.0120 (9) | −0.0122 (8) | −0.0012 (8) |
| O3 | 0.0504 (14) | 0.0431 (12) | 0.1041 (18) | −0.0248 (11) | −0.0063 (13) | −0.0148 (13) |
| O3W | 0.0596 (15) | 0.0539 (14) | 0.0622 (14) | −0.0233 (12) | −0.0267 (12) | 0.0194 (10) |
| O4 | 0.0361 (11) | 0.0234 (10) | 0.0840 (14) | −0.0116 (8) | −0.0223 (10) | 0.0096 (9) |
| O5 | 0.0338 (10) | 0.0245 (9) | 0.0676 (12) | −0.0076 (8) | −0.0240 (9) | −0.0043 (8) |
| O6 | 0.0937 (17) | 0.0321 (11) | 0.0460 (11) | −0.0266 (11) | −0.0135 (11) | 0.0007 (9) |
| O7 | 0.0681 (13) | 0.0516 (12) | 0.0371 (10) | −0.0444 (11) | −0.0149 (9) | 0.0063 (8) |
| O8 | 0.0360 (10) | 0.0230 (8) | 0.0345 (9) | −0.0143 (8) | −0.0084 (8) | 0.0035 (7) |
| O9 | 0.0591 (14) | 0.0370 (11) | 0.0821 (15) | −0.0156 (10) | −0.0386 (12) | 0.0092 (10) |
| O10 | 0.0338 (10) | 0.0220 (8) | 0.0348 (9) | −0.0132 (7) | −0.0099 (7) | 0.0045 (7) |
| O11 | 0.0513 (11) | 0.0341 (10) | 0.0368 (9) | −0.0265 (9) | −0.0169 (8) | 0.0075 (8) |
| O12 | 0.0506 (12) | 0.0342 (10) | 0.0549 (12) | −0.0208 (9) | −0.0137 (9) | 0.0130 (9) |
| O13 | 0.0274 (10) | 0.0226 (9) | 0.0656 (12) | −0.0073 (8) | −0.0146 (9) | −0.0041 (8) |
| O14 | 0.0317 (10) | 0.0221 (9) | 0.0688 (13) | −0.0078 (8) | −0.0090 (9) | 0.0015 (8) |
| O15 | 0.0797 (15) | 0.0260 (10) | 0.0565 (12) | −0.0175 (10) | −0.0229 (11) | 0.0009 (9) |
| O16 | 0.0387 (11) | 0.0405 (11) | 0.0439 (10) | −0.0121 (9) | −0.0120 (9) | −0.0053 (8) |
| O17 | 0.0501 (13) | 0.0438 (11) | 0.0433 (11) | 0.0028 (10) | −0.0203 (10) | −0.0081 (9) |
| O18 | 0.0785 (17) | 0.0333 (12) | 0.116 (2) | −0.0211 (12) | −0.0315 (15) | −0.0007 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Nd1—O4 | 2.4611 (17) | C28—O12 | 1.376 (3) |
| Nd1—O5 | 2.4624 (16) | C28—C29 | 1.377 (4) |
| Nd1—O10 | 2.4666 (15) | C29—C30 | 1.379 (4) |
| Nd1—O1W | 2.4820 (16) | C29—H29A | 0.9300 |
| Nd1—O2 | 2.4829 (17) | C30—H30A | 0.9300 |
| Nd1—O7 | 2.5033 (17) | C31—C32 | 1.508 (3) |
| Nd1—O1 | 2.5724 (16) | C31—H31A | 0.9700 |
| Nd1—O8 | 2.6104 (15) | C31—H31B | 0.9700 |
| Nd1—N1 | 2.6326 (19) | C32—O11 | 1.251 (3) |
| Nd1—C16 | 2.816 (2) | C32—O10 | 1.269 (3) |
| Nd1—C8 | 2.899 (2) | C33—C38 | 1.385 (3) |
| Nd1—C24 | 2.921 (2) | C33—C34 | 1.387 (3) |
| Nd2—O8 | 2.4179 (15) | C33—C39 | 1.501 (3) |
| Nd2—O14 | 2.4506 (17) | C34—C35 | 1.367 (3) |
| Nd2—O13 | 2.4640 (16) | C34—H34A | 0.9300 |
| Nd2—O2W | 2.4793 (16) | C35—C36 | 1.383 (3) |
| Nd2—O16 | 2.4978 (17) | C35—H35A | 0.9300 |
| Nd2—O17 | 2.5552 (17) | C36—O15 | 1.359 (3) |
| Nd2—O10 | 2.5845 (15) | C36—C37 | 1.381 (4) |
| Nd2—O11 | 2.6236 (16) | C37—C38 | 1.383 (3) |
| Nd2—N3 | 2.6545 (18) | C37—H37A | 0.9300 |
| Nd2—C40 | 2.838 (2) | C38—H38A | 0.9300 |
| Nd2—C48 | 2.899 (2) | C39—C40 | 1.498 (3) |
| Nd2—C32 | 2.976 (2) | C39—H39A | 0.9700 |
| N1—C49 | 1.330 (3) | C39—H39B | 0.9700 |
| N1—C53 | 1.332 (3) | C40—O14 | 1.257 (3) |
| N2—C58 | 1.313 (4) | C40—O13 | 1.269 (3) |
| N2—C54 | 1.329 (4) | C41—C46 | 1.388 (4) |
| N3—C59 | 1.330 (3) | C41—C42 | 1.391 (4) |
| N3—C63 | 1.337 (3) | C41—C47 | 1.509 (3) |
| N4—C64 | 1.322 (5) | C42—C43 | 1.373 (4) |
| N4—C68 | 1.328 (5) | C42—H42A | 0.9300 |
| C1—C2 | 1.378 (4) | C43—C44 | 1.379 (4) |
| C1—C6 | 1.387 (3) | C43—H43A | 0.9300 |
| C1—C7 | 1.513 (3) | C44—O18 | 1.367 (3) |
| C2—C3 | 1.384 (4) | C44—C45 | 1.377 (4) |
| C2—H2A | 0.9300 | C45—C46 | 1.379 (4) |
| C3—C4 | 1.369 (4) | C45—H45A | 0.9300 |
| C3—H3A | 0.9300 | C46—H46A | 0.9300 |
| C4—C5 | 1.372 (4) | C47—C48 | 1.515 (3) |
| C4—O3 | 1.379 (3) | C47—H47A | 0.9700 |
| C5—C6 | 1.374 (4) | C47—H47B | 0.9700 |
| C5—H5A | 0.9300 | C48—O16 | 1.248 (3) |
| C6—H6A | 0.9300 | C48—O17 | 1.262 (3) |
| C7—C8 | 1.508 (3) | C49—C50 | 1.383 (3) |
| C7—H7A | 0.9700 | C49—H49A | 0.9300 |

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| C7—H7B | 0.9700 | C50—C51 | 1.382 (4) |
| C8—O2 | 1.255 (3) | C50—H50A | 0.9300 |
| C8—O1 | 1.262 (3) | C51—C52 | 1.384 (4) |
| C9—C10 | 1.371 (4) | C51—C56 | 1.486 (3) |
| C9—C14 | 1.392 (3) | C52—C53 | 1.376 (3) |
| C9—C15 | 1.501 (3) | C52—H52A | 0.9300 |
| C10—C11 | 1.382 (4) | C53—H53A | 0.9300 |
| C10—H10A | 0.9300 | C54—C55 | 1.383 (4) |
| C11—C12 | 1.369 (3) | C54—H54A | 0.9300 |
| C11—H11A | 0.9300 | C55—C56 | 1.378 (4) |
| C12—O6 | 1.370 (3) | C55—H55A | 0.9300 |
| C12—C13 | 1.381 (3) | C56—C57 | 1.380 (4) |
| C13—C14 | 1.363 (3) | C57—C58 | 1.386 (4) |
| C13—H13A | 0.9300 | C57—H57A | 0.9300 |
| C14—H14A | 0.9300 | C58—H58A | 0.9300 |
| C15—C16 | 1.509 (3) | C59—C60 | 1.381 (3) |
| C15—H15A | 0.9700 | C59—H59A | 0.9300 |
| C15—H15B | 0.9700 | C60—C61 | 1.380 (4) |
| C16—O4 | 1.254 (3) | C60—H60A | 0.9300 |
| C16—O5 | 1.262 (3) | C61—C62 | 1.391 (4) |
| C17—C18 | 1.377 (4) | C61—C66 | 1.483 (3) |
| C17—C22 | 1.382 (4) | C62—C63 | 1.377 (3) |
| C17—C23 | 1.505 (4) | C62—H62A | 0.9300 |
| C18—C19 | 1.387 (4) | C63—H63A | 0.9300 |
| C18—H18A | 0.9300 | C64—C65 | 1.380 (4) |
| C19—C20 | 1.380 (4) | C64—H64A | 0.9300 |
| C19—H19A | 0.9300 | C65—C66 | 1.386 (4) |
| C20—O9 | 1.373 (3) | C65—H65A | 0.9300 |
| C20—C21 | 1.378 (4) | C66—C67 | 1.386 (4) |
| C21—C22 | 1.376 (3) | C67—C68 | 1.383 (4) |
| C21—H21A | 0.9300 | C67—H67A | 0.9300 |
| C22—H22A | 0.9300 | C68—H68A | 0.9300 |
| C23—C24 | 1.509 (3) | O1W—H1WA | 0.81 (2) |
| C23—H23A | 0.9700 | O1W—H1WB | 0.82 (2) |
| C23—H23B | 0.9700 | O2W—H2WA | 0.82 (2) |
| C24—O7 | 1.238 (3) | O2W—H2WB | 0.81 (2) |
| C24—O8 | 1.269 (3) | O3—H3B | 0.8200 |
| C25—C30 | 1.376 (4) | O3W—H3WA | 0.82 (2) |
| C25—C26 | 1.388 (4) | O3W—H3WB | 0.82 (2) |
| C25—C31 | 1.506 (3) | O6—H6B | 0.8200 |
| C26—C27 | 1.386 (3) | O9—H9A | 0.8200 |
| C26—H26A | 0.9300 | O12—H12A | 0.8200 |
| C27—C28 | 1.377 (4) | O15—H15C | 0.8200 |
| C27—H27A | 0.9300 | O18—H18B | 0.8200 |
| | | | |
| O4—Nd1—O5 | 52.77 (5) | C19—C18—H18A | 119.0 |
| O4—Nd1—O10 | 125.18 (5) | C20—C19—C18 | 119.2 (3) |
| O5—Nd1—O10 | 72.80 (5) | C20—C19—H19A | 120.4 |

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| O4—Nd1—O1W | 151.17 (6) | C18—C19—H19A | 120.4 |
| O5—Nd1—O1W | 144.97 (5) | O9—C20—C21 | 117.9 (2) |
| O10—Nd1—O1W | 79.96 (5) | O9—C20—C19 | 122.4 (3) |
| O4—Nd1—O2 | 116.30 (6) | C21—C20—C19 | 119.7 (2) |
| O5—Nd1—O2 | 123.58 (6) | C22—C21—C20 | 119.9 (3) |
| O10—Nd1—O2 | 86.53 (5) | C22—C21—H21A | 120.0 |
| O1W—Nd1—O2 | 75.10 (6) | C20—C21—H21A | 120.0 |
| O4—Nd1—O7 | 77.79 (6) | C21—C22—C17 | 121.6 (3) |
| O5—Nd1—O7 | 95.05 (6) | C21—C22—H22A | 119.2 |
| O10—Nd1—O7 | 116.73 (5) | C17—C22—H22A | 119.2 |
| O1W—Nd1—O7 | 77.80 (7) | C17—C23—C24 | 112.3 (2) |
| O2—Nd1—O7 | 140.21 (6) | C17—C23—H23A | 109.1 |
| O4—Nd1—O1 | 73.13 (6) | C24—C23—H23A | 109.1 |
| O5—Nd1—O1 | 76.34 (6) | C17—C23—H23B | 109.1 |
| O10—Nd1—O1 | 89.72 (5) | C24—C23—H23B | 109.1 |
| O1W—Nd1—O1 | 125.79 (6) | H23A—C23—H23B | 107.9 |
| O2—Nd1—O1 | 51.08 (6) | O7—C24—O8 | 121.1 (2) |
| O7—Nd1—O1 | 148.77 (6) | O7—C24—C23 | 119.8 (2) |
| O4—Nd1—O8 | 102.01 (6) | O8—C24—C23 | 119.1 (2) |
| O5—Nd1—O8 | 75.76 (5) | O7—C24—Nd1 | 58.32 (12) |
| O10—Nd1—O8 | 66.52 (5) | O8—C24—Nd1 | 63.32 (12) |
| O1W—Nd1—O8 | 73.40 (5) | C23—C24—Nd1 | 171.22 (19) |
| O2—Nd1—O8 | 141.38 (5) | C30—C25—C26 | 117.8 (2) |
| O7—Nd1—O8 | 50.48 (5) | C30—C25—C31 | 120.5 (3) |
| O1—Nd1—O8 | 147.63 (5) | C26—C25—C31 | 121.7 (3) |
| O4—Nd1—N1 | 76.87 (6) | C27—C26—C25 | 121.2 (3) |
| O5—Nd1—N1 | 129.58 (6) | C27—C26—H26A | 119.4 |
| O10—Nd1—N1 | 155.81 (6) | C25—C26—H26A | 119.4 |
| O1W—Nd1—N1 | 82.04 (6) | C28—C27—C26 | 119.5 (2) |
| O2—Nd1—N1 | 73.28 (6) | C28—C27—H27A | 120.3 |
| O7—Nd1—N1 | 74.58 (6) | C26—C27—H27A | 120.3 |
| O1—Nd1—N1 | 87.81 (6) | O12—C28—C29 | 117.8 (2) |
| O8—Nd1—N1 | 122.92 (5) | O12—C28—C27 | 122.0 (2) |
| O4—Nd1—C16 | 26.40 (6) | C29—C28—C27 | 120.2 (2) |
| O5—Nd1—C16 | 26.59 (6) | C28—C29—C30 | 119.4 (3) |
| O10—Nd1—C16 | 98.80 (6) | C28—C29—H29A | 120.3 |
| O1W—Nd1—C16 | 163.55 (7) | C30—C29—H29A | 120.3 |
| O2—Nd1—C16 | 121.30 (6) | C25—C30—C29 | 121.9 (3) |
| O7—Nd1—C16 | 88.36 (7) | C25—C30—H30A | 119.1 |
| O1—Nd1—C16 | 70.42 (6) | C29—C30—H30A | 119.1 |
| O8—Nd1—C16 | 90.98 (6) | C25—C31—C32 | 114.9 (2) |
| N1—Nd1—C16 | 102.99 (7) | C25—C31—H31A | 108.5 |
| O4—Nd1—C8 | 93.67 (7) | C32—C31—H31A | 108.5 |
| O5—Nd1—C8 | 101.18 (7) | C25—C31—H31B | 108.5 |
| O10—Nd1—C8 | 90.43 (6) | C32—C31—H31B | 108.5 |
| O1W—Nd1—C8 | 100.61 (7) | H31A—C31—H31B | 107.5 |
| O2—Nd1—C8 | 25.51 (6) | O11—C32—O10 | 120.3 (2) |
| O7—Nd1—C8 | 151.62 (6) | O11—C32—C31 | 122.4 (2) |

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| O1—Nd1—C8 | 25.81 (6) | O10—C32—C31 | 117.2 (2) |
| O8—Nd1—C8 | 156.75 (6) | O11—C32—Nd2 | 61.64 (12) |
| N1—Nd1—C8 | 77.14 (6) | O10—C32—Nd2 | 59.91 (11) |
| C16—Nd1—C8 | 95.80 (7) | C31—C32—Nd2 | 168.17 (18) |
| O4—Nd1—C24 | 91.45 (7) | C38—C33—C34 | 117.0 (2) |
| O5—Nd1—C24 | 87.01 (6) | C38—C33—C39 | 121.6 (2) |
| O10—Nd1—C24 | 91.85 (6) | C34—C33—C39 | 121.4 (2) |
| O1W—Nd1—C24 | 72.08 (7) | C35—C34—C33 | 122.1 (2) |
| O2—Nd1—C24 | 146.91 (6) | C35—C34—H34A | 118.9 |
| O7—Nd1—C24 | 24.89 (6) | C33—C34—H34A | 118.9 |
| O1—Nd1—C24 | 162.01 (7) | C34—C35—C36 | 120.3 (2) |
| O8—Nd1—C24 | 25.74 (6) | C34—C35—H35A | 119.9 |
| N1—Nd1—C24 | 97.85 (6) | C36—C35—H35A | 119.9 |
| C16—Nd1—C24 | 91.63 (7) | O15—C36—C37 | 123.1 (2) |
| C8—Nd1—C24 | 171.81 (7) | O15—C36—C35 | 118.1 (2) |
| O8—Nd2—O14 | 127.17 (5) | C37—C36—C35 | 118.8 (2) |
| O8—Nd2—O13 | 74.96 (5) | C36—C37—C38 | 120.2 (2) |
| O14—Nd2—O13 | 52.73 (5) | C36—C37—H37A | 119.9 |
| O8—Nd2—O2W | 78.76 (6) | C38—C37—H37A | 119.9 |
| O14—Nd2—O2W | 144.15 (6) | C37—C38—C33 | 121.5 (2) |
| O13—Nd2—O2W | 147.27 (5) | C37—C38—H38A | 119.3 |
| O8—Nd2—O16 | 81.88 (5) | C33—C38—H38A | 119.3 |
| O14—Nd2—O16 | 126.32 (6) | C40—C39—C33 | 116.0 (2) |
| O13—Nd2—O16 | 118.12 (6) | C40—C39—H39A | 108.3 |
| O2W—Nd2—O16 | 76.34 (6) | C33—C39—H39A | 108.3 |
| O8—Nd2—O17 | 97.95 (6) | C40—C39—H39B | 108.3 |
| O14—Nd2—O17 | 78.44 (6) | C33—C39—H39B | 108.3 |
| O13—Nd2—O17 | 76.46 (6) | H39A—C39—H39B | 107.4 |
| O2W—Nd2—O17 | 126.81 (6) | O14—C40—O13 | 119.5 (2) |
| O16—Nd2—O17 | 50.94 (6) | O14—C40—C39 | 119.3 (2) |
| O8—Nd2—O10 | 67.63 (5) | O13—C40—C39 | 121.2 (2) |
| O14—Nd2—O10 | 90.57 (5) | O14—C40—Nd2 | 59.44 (12) |
| O13—Nd2—O10 | 75.76 (5) | O13—C40—Nd2 | 60.09 (12) |
| O2W—Nd2—O10 | 76.42 (6) | C39—C40—Nd2 | 177.45 (16) |
| O16—Nd2—O10 | 142.31 (5) | C46—C41—C42 | 117.2 (2) |
| O17—Nd2—O10 | 151.23 (5) | C46—C41—C47 | 120.7 (3) |
| O8—Nd2—O11 | 114.99 (5) | C42—C41—C47 | 122.1 (2) |
| O14—Nd2—O11 | 73.64 (6) | C43—C42—C41 | 122.0 (2) |
| O13—Nd2—O11 | 101.41 (6) | C43—C42—H42A | 119.0 |
| O2W—Nd2—O11 | 72.54 (6) | C41—C42—H42A | 119.0 |
| O16—Nd2—O11 | 140.16 (6) | C42—C43—C44 | 119.6 (3) |
| O17—Nd2—O11 | 145.48 (6) | C42—C43—H43A | 120.2 |
| O10—Nd2—O11 | 49.63 (5) | C44—C43—H43A | 120.2 |
| O8—Nd2—N3 | 155.81 (6) | O18—C44—C45 | 122.9 (3) |
| O14—Nd2—N3 | 75.75 (6) | O18—C44—C43 | 117.5 (3) |
| O13—Nd2—N3 | 125.68 (6) | C45—C44—C43 | 119.6 (3) |
| O2W—Nd2—N3 | 84.93 (6) | C44—C45—C46 | 120.3 (3) |
| O16—Nd2—N3 | 76.96 (6) | C44—C45—H45A | 119.8 |

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| O17—Nd2—N3 | 77.67 (6) | C46—C45—H45A | 119.8 |
| O10—Nd2—N3 | 125.60 (5) | C45—C46—C41 | 121.2 (3) |
| O11—Nd2—N3 | 76.11 (5) | C45—C46—H46A | 119.4 |
| O8—Nd2—C40 | 101.29 (6) | C41—C46—H46A | 119.4 |
| O14—Nd2—C40 | 26.21 (6) | C41—C47—C48 | 112.0 (2) |
| O13—Nd2—C40 | 26.52 (6) | C41—C47—H47A | 109.2 |
| O2W—Nd2—C40 | 157.53 (7) | C48—C47—H47A | 109.2 |
| O16—Nd2—C40 | 126.09 (6) | C41—C47—H47B | 109.2 |
| O17—Nd2—C40 | 75.62 (6) | C48—C47—H47B | 109.2 |
| O10—Nd2—C40 | 82.81 (6) | H47A—C47—H47B | 107.9 |
| O11—Nd2—C40 | 87.53 (6) | O16—C48—O17 | 120.0 (2) |
| N3—Nd2—C40 | 100.59 (6) | O16—C48—C47 | 119.8 (2) |
| O8—Nd2—C48 | 92.04 (6) | O17—C48—C47 | 120.2 (2) |
| O14—Nd2—C48 | 101.96 (7) | O16—C48—Nd2 | 59.05 (13) |
| O13—Nd2—C48 | 99.02 (7) | O17—C48—Nd2 | 61.72 (12) |
| O2W—Nd2—C48 | 101.08 (7) | C47—C48—Nd2 | 170.41 (17) |
| O16—Nd2—C48 | 25.36 (6) | N1—C49—C50 | 123.1 (2) |
| O17—Nd2—C48 | 25.78 (6) | N1—C49—H49A | 118.5 |
| O10—Nd2—C48 | 159.65 (6) | C50—C49—H49A | 118.5 |
| O11—Nd2—C48 | 149.50 (6) | C51—C50—C49 | 119.7 (2) |
| N3—Nd2—C48 | 73.60 (6) | C51—C50—H50A | 120.1 |
| C40—Nd2—C48 | 101.38 (7) | C49—C50—H50A | 120.1 |
| O8—Nd2—C32 | 90.62 (6) | C50—C51—C52 | 117.0 (2) |
| O14—Nd2—C32 | 84.08 (6) | C50—C51—C56 | 121.4 (2) |
| O13—Nd2—C32 | 91.06 (6) | C52—C51—C56 | 121.5 (2) |
| O2W—Nd2—C32 | 69.93 (7) | C53—C52—C51 | 119.6 (2) |
| O16—Nd2—C32 | 146.25 (6) | C53—C52—H52A | 120.2 |
| O17—Nd2—C32 | 162.35 (6) | C51—C52—H52A | 120.2 |
| O10—Nd2—C32 | 25.13 (5) | N1—C53—C52 | 123.4 (2) |
| O11—Nd2—C32 | 24.82 (5) | N1—C53—H53A | 118.3 |
| N3—Nd2—C32 | 100.48 (6) | C52—C53—H53A | 118.3 |
| C40—Nd2—C32 | 87.62 (6) | N2—C54—C55 | 123.9 (3) |
| C48—Nd2—C32 | 169.92 (7) | N2—C54—H54A | 118.0 |
| C49—N1—C53 | 117.1 (2) | C55—C54—H54A | 118.0 |
| C49—N1—Nd1 | 124.12 (16) | C56—C55—C54 | 119.4 (3) |
| C53—N1—Nd1 | 118.35 (16) | C56—C55—H55A | 120.3 |
| C58—N2—C54 | 116.0 (3) | C54—C55—H55A | 120.3 |
| C59—N3—C63 | 116.8 (2) | C55—C56—C57 | 117.0 (3) |
| C59—N3—Nd2 | 121.34 (16) | C55—C56—C51 | 121.2 (3) |
| C63—N3—Nd2 | 121.34 (15) | C57—C56—C51 | 121.7 (3) |
| C64—N4—C68 | 115.9 (3) | C56—C57—C58 | 119.0 (3) |
| C2—C1—C6 | 117.6 (2) | C56—C57—H57A | 120.5 |
| C2—C1—C7 | 122.0 (2) | C58—C57—H57A | 120.5 |
| C6—C1—C7 | 120.4 (2) | N2—C58—C57 | 124.6 (3) |
| C1—C2—C3 | 121.5 (3) | N2—C58—H58A | 117.7 |
| C1—C2—H2A | 119.3 | C57—C58—H58A | 117.7 |
| C3—C2—H2A | 119.3 | N3—C59—C60 | 123.2 (2) |
| C4—C3—C2 | 119.7 (3) | N3—C59—H59A | 118.4 |

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| C4—C3—H3A | 120.1 | C60—C59—H59A | 118.4 |
| C2—C3—H3A | 120.1 | C61—C60—C59 | 120.4 (2) |
| C3—C4—C5 | 119.8 (3) | C61—C60—H60A | 119.8 |
| C3—C4—O3 | 118.5 (3) | C59—C60—H60A | 119.8 |
| C5—C4—O3 | 121.7 (3) | C60—C61—C62 | 116.1 (2) |
| C4—C5—C6 | 120.2 (3) | C60—C61—C66 | 121.3 (2) |
| C4—C5—H5A | 119.9 | C62—C61—C66 | 122.5 (2) |
| C6—C5—H5A | 119.9 | C63—C62—C61 | 120.1 (2) |
| C5—C6—C1 | 121.2 (3) | C63—C62—H62A | 119.9 |
| C5—C6—H6A | 119.4 | C61—C62—H62A | 119.9 |
| C1—C6—H6A | 119.4 | N3—C63—C62 | 123.3 (2) |
| C8—C7—C1 | 111.7 (2) | N3—C63—H63A | 118.4 |
| C8—C7—H7A | 109.3 | C62—C63—H63A | 118.4 |
| C1—C7—H7A | 109.3 | N4—C64—C65 | 124.3 (3) |
| C8—C7—H7B | 109.3 | N4—C64—H64A | 117.9 |
| C1—C7—H7B | 109.3 | C65—C64—H64A | 117.9 |
| H7A—C7—H7B | 107.9 | C64—C65—C66 | 119.7 (3) |
| O2—C8—O1 | 120.1 (2) | C64—C65—H65A | 120.2 |
| O2—C8—C7 | 119.6 (2) | C66—C65—H65A | 120.2 |
| O1—C8—C7 | 120.3 (2) | C67—C66—C65 | 116.4 (3) |
| O2—C8—Nd1 | 58.40 (12) | C67—C66—C61 | 121.3 (3) |
| O1—C8—Nd1 | 62.51 (12) | C65—C66—C61 | 122.3 (3) |
| C7—C8—Nd1 | 168.90 (16) | C68—C67—C66 | 119.4 (3) |
| C10—C9—C14 | 117.0 (2) | C68—C67—H67A | 120.3 |
| C10—C9—C15 | 122.1 (2) | C66—C67—H67A | 120.3 |
| C14—C9—C15 | 120.9 (2) | N4—C68—C67 | 124.3 (4) |
| C9—C10—C11 | 122.2 (2) | N4—C68—H68A | 117.9 |
| C9—C10—H10A | 118.9 | C67—C68—H68A | 117.9 |
| C11—C10—H10A | 118.9 | Nd1—O1W—H1WA | 118.6 (19) |
| C12—C11—C10 | 119.6 (2) | Nd1—O1W—H1WB | 135.0 (19) |
| C12—C11—H11A | 120.2 | H1WA—O1W—H1WB | 106 (2) |
| C10—C11—H11A | 120.2 | C8—O1—Nd1 | 91.69 (14) |
| C11—C12—O6 | 123.2 (2) | Nd2—O2W—H2WA | 122.1 (19) |
| C11—C12—C13 | 119.3 (2) | Nd2—O2W—H2WB | 130 (2) |
| O6—C12—C13 | 117.5 (2) | H2WA—O2W—H2WB | 108 (2) |
| C14—C13—C12 | 120.3 (2) | C8—O2—Nd1 | 96.09 (15) |
| C14—C13—H13A | 119.8 | C4—O3—H3B | 109.5 |
| C12—C13—H13A | 119.8 | H3WA—O3W—H3WB | 106 (2) |
| C13—C14—C9 | 121.5 (2) | C16—O4—Nd1 | 92.81 (14) |
| C13—C14—H14A | 119.2 | C16—O5—Nd1 | 92.54 (14) |
| C9—C14—H14A | 119.2 | C12—O6—H6B | 109.5 |
| C9—C15—C16 | 115.3 (2) | C24—O7—Nd1 | 96.79 (14) |
| C9—C15—H15A | 108.4 | C24—O8—Nd2 | 153.48 (15) |
| C16—C15—H15A | 108.4 | C24—O8—Nd1 | 90.94 (13) |
| C9—C15—H15B | 108.4 | Nd2—O8—Nd1 | 113.30 (6) |
| C16—C15—H15B | 108.4 | C20—O9—H9A | 109.5 |
| H15A—C15—H15B | 107.5 | C32—O10—Nd1 | 143.18 (14) |
| O4—C16—O5 | 120.9 (2) | C32—O10—Nd2 | 94.95 (13) |

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| O4—C16—C15 | 118.9 (2) | Nd1—O10—Nd2 | 112.55 (6) |
| O5—C16—C15 | 120.1 (2) | C32—O11—Nd2 | 93.55 (13) |
| O4—C16—Nd1 | 60.79 (13) | C28—O12—H12A | 109.5 |
| O5—C16—Nd1 | 60.87 (12) | C40—O13—Nd2 | 93.39 (13) |
| C15—C16—Nd1 | 168.94 (19) | C40—O14—Nd2 | 94.34 (14) |
| C18—C17—C22 | 117.5 (3) | C36—O15—H15C | 109.5 |
| C18—C17—C23 | 121.0 (3) | C48—O16—Nd2 | 95.59 (15) |
| C22—C17—C23 | 121.4 (3) | C48—O17—Nd2 | 92.50 (14) |
| C17—C18—C19 | 121.9 (3) | C44—O18—H18B | 109.5 |
| C17—C18—H18A | 119.0 | | |

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| O4—Nd1—N1—C49 | −148.29 (19) | O14—Nd2—C48—O16 | −165.18 (13) |
| O5—Nd1—N1—C49 | −145.32 (17) | O13—Nd2—C48—O16 | 141.20 (14) |
| O10—Nd1—N1—C49 | 9.3 (3) | O2W—Nd2—C48—O16 | −12.84 (15) |
| O1W—Nd1—N1—C49 | 51.50 (18) | O17—Nd2—C48—O16 | 170.3 (2) |
| O2—Nd1—N1—C49 | −25.26 (18) | O10—Nd2—C48—O16 | 67.9 (2) |
| O7—Nd1—N1—C49 | 130.97 (19) | O11—Nd2—C48—O16 | −87.18 (19) |
| O1—Nd1—N1—C49 | −75.10 (19) | N3—Nd2—C48—O16 | −94.13 (14) |
| O8—Nd1—N1—C49 | 115.77 (18) | C40—Nd2—C48—O16 | 168.05 (14) |
| C16—Nd1—N1—C49 | −144.43 (18) | C32—Nd2—C48—O16 | −39.1 (4) |
| C8—Nd1—N1—C49 | −51.35 (19) | O8—Nd2—C48—O17 | −104.16 (15) |
| C24—Nd1—N1—C49 | 122.06 (19) | O14—Nd2—C48—O17 | 24.56 (15) |
| O4—Nd1—N1—C53 | 39.24 (18) | O13—Nd2—C48—O17 | −29.06 (15) |
| O5—Nd1—N1—C53 | 42.2 (2) | O2W—Nd2—C48—O17 | 176.90 (14) |
| O10—Nd1—N1—C53 | −163.16 (16) | O16—Nd2—C48—O17 | −170.3 (2) |
| O1W—Nd1—N1—C53 | −120.97 (19) | O10—Nd2—C48—O17 | −102.3 (2) |
| O2—Nd1—N1—C53 | 162.27 (19) | O11—Nd2—C48—O17 | 102.57 (17) |
| O7—Nd1—N1—C53 | −41.51 (18) | N3—Nd2—C48—O17 | 95.61 (15) |
| O1—Nd1—N1—C53 | 112.43 (18) | C40—Nd2—C48—O17 | −2.21 (16) |
| O8—Nd1—N1—C53 | −56.71 (19) | C32—Nd2—C48—O17 | 150.7 (3) |
| C16—Nd1—N1—C53 | 43.09 (19) | O8—Nd2—C48—C47 | 151.8 (12) |
| C8—Nd1—N1—C53 | 136.17 (19) | O14—Nd2—C48—C47 | −79.5 (12) |
| C24—Nd1—N1—C53 | −50.42 (18) | O13—Nd2—C48—C47 | −133.1 (12) |
| O8—Nd2—N3—C59 | 0.7 (3) | O2W—Nd2—C48—C47 | 72.9 (12) |
| O14—Nd2—N3—C59 | 163.59 (19) | O16—Nd2—C48—C47 | 85.7 (12) |
| O13—Nd2—N3—C59 | 145.70 (17) | O17—Nd2—C48—C47 | −104.0 (12) |
| O2W—Nd2—N3—C59 | −46.85 (18) | O10—Nd2—C48—C47 | 153.7 (11) |
| O16—Nd2—N3—C59 | 30.27 (17) | O11—Nd2—C48—C47 | −1.4 (13) |
| O17—Nd2—N3—C59 | 82.57 (18) | N3—Nd2—C48—C47 | −8.4 (12) |
| O10—Nd2—N3—C59 | −116.15 (17) | C40—Nd2—C48—C47 | −106.2 (12) |
| O11—Nd2—N3—C59 | −120.09 (18) | C32—Nd2—C48—C47 | 46.6 (14) |
| C40—Nd2—N3—C59 | 155.15 (18) | C53—N1—C49—C50 | 1.8 (4) |
| C48—Nd2—N3—C59 | 56.28 (18) | Nd1—N1—C49—C50 | −170.76 (18) |
| C32—Nd2—N3—C59 | −115.33 (18) | N1—C49—C50—C51 | 0.2 (4) |
| O8—Nd2—N3—C63 | 171.95 (15) | C49—C50—C51—C52 | −1.8 (4) |
| O14—Nd2—N3—C63 | −25.13 (17) | C49—C50—C51—C56 | 176.3 (2) |
| O13—Nd2—N3—C63 | −43.03 (19) | C50—C51—C52—C53 | 1.4 (4) |
| O2W—Nd2—N3—C63 | 124.42 (18) | C56—C51—C52—C53 | −176.6 (2) |

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| O16—Nd2—N3—C63 | −158.45 (18) | C49—N1—C53—C52 | −2.2 (4) |
| O17—Nd2—N3—C63 | −106.15 (18) | Nd1—N1—C53—C52 | 170.8 (2) |
| O10—Nd2—N3—C63 | 55.12 (19) | C51—C52—C53—N1 | 0.6 (4) |
| O11—Nd2—N3—C63 | 51.18 (17) | C58—N2—C54—C55 | 0.9 (5) |
| C40—Nd2—N3—C63 | −33.58 (18) | N2—C54—C55—C56 | 0.2 (5) |
| C48—Nd2—N3—C63 | −132.45 (19) | C54—C55—C56—C57 | −1.5 (4) |
| C32—Nd2—N3—C63 | 55.94 (18) | C54—C55—C56—C51 | 176.0 (3) |
| C6—C1—C2—C3 | −1.7 (4) | C50—C51—C56—C55 | −148.1 (3) |
| C7—C1—C2—C3 | −179.1 (2) | C52—C51—C56—C55 | 29.8 (4) |
| C1—C2—C3—C4 | 1.2 (4) | C50—C51—C56—C57 | 29.3 (4) |
| C2—C3—C4—C5 | 0.9 (4) | C52—C51—C56—C57 | −152.7 (3) |
| C2—C3—C4—O3 | −179.6 (3) | C55—C56—C57—C58 | 1.8 (4) |
| C3—C4—C5—C6 | −2.4 (4) | C51—C56—C57—C58 | −175.7 (3) |
| O3—C4—C5—C6 | 178.2 (3) | C54—N2—C58—C57 | −0.6 (5) |
| C4—C5—C6—C1 | 1.8 (4) | C56—C57—C58—N2 | −0.8 (5) |
| C2—C1—C6—C5 | 0.2 (4) | C63—N3—C59—C60 | −2.0 (4) |
| C7—C1—C6—C5 | 177.7 (2) | Nd2—N3—C59—C60 | 169.66 (18) |
| C2—C1—C7—C8 | −49.4 (3) | N3—C59—C60—C61 | −1.0 (4) |
| C6—C1—C7—C8 | 133.2 (3) | C59—C60—C61—C62 | 3.0 (4) |
| C1—C7—C8—O2 | −77.0 (3) | C59—C60—C61—C66 | −174.1 (2) |
| C1—C7—C8—O1 | 101.1 (3) | C60—C61—C62—C63 | −2.0 (4) |
| C1—C7—C8—Nd1 | −0.3 (11) | C66—C61—C62—C63 | 175.0 (2) |
| O4—Nd1—C8—O2 | 153.70 (14) | C59—N3—C63—C62 | 3.0 (4) |
| O5—Nd1—C8—O2 | −153.55 (13) | Nd2—N3—C63—C62 | −168.67 (18) |
| O10—Nd1—C8—O2 | −81.01 (14) | C61—C62—C63—N3 | −1.0 (4) |
| O1W—Nd1—C8—O2 | −1.15 (14) | C68—N4—C64—C65 | 0.5 (5) |
| O7—Nd1—C8—O2 | 82.8 (2) | N4—C64—C65—C66 | 1.3 (5) |
| O1—Nd1—C8—O2 | −169.5 (2) | C64—C65—C66—C67 | −1.6 (4) |
| O8—Nd1—C8—O2 | −73.7 (2) | C64—C65—C66—C61 | 175.0 (3) |
| N1—Nd1—C8—O2 | 78.06 (14) | C60—C61—C66—C67 | 159.8 (3) |
| C16—Nd1—C8—O2 | −179.90 (14) | C62—C61—C66—C67 | −17.1 (4) |
| C24—Nd1—C8—O2 | 25.1 (5) | C60—C61—C66—C65 | −16.6 (4) |
| O4—Nd1—C8—O1 | −36.83 (14) | C62—C61—C66—C65 | 166.5 (3) |
| O5—Nd1—C8—O1 | 15.93 (15) | C65—C66—C67—C68 | 0.3 (4) |
| O10—Nd1—C8—O1 | 88.47 (14) | C61—C66—C67—C68 | −176.3 (3) |
| O1W—Nd1—C8—O1 | 168.33 (14) | C64—N4—C68—C67 | −1.9 (5) |
| O2—Nd1—C8—O1 | 169.5 (2) | C66—C67—C68—N4 | 1.6 (5) |
| O7—Nd1—C8—O1 | −107.74 (18) | O2—C8—O1—Nd1 | 10.4 (2) |
| O8—Nd1—C8—O1 | 95.8 (2) | C7—C8—O1—Nd1 | −167.7 (2) |
| N1—Nd1—C8—O1 | −112.46 (15) | O4—Nd1—O1—C8 | 141.32 (15) |
| C16—Nd1—C8—O1 | −10.42 (15) | O5—Nd1—O1—C8 | −163.92 (15) |
| C24—Nd1—C8—O1 | −165.4 (4) | O10—Nd1—O1—C8 | −91.56 (14) |
| O4—Nd1—C8—C7 | 70.6 (10) | O1W—Nd1—O1—C8 | −14.19 (17) |
| O5—Nd1—C8—C7 | 123.3 (10) | O2—Nd1—O1—C8 | −5.80 (13) |
| O10—Nd1—C8—C7 | −164.1 (10) | O7—Nd1—O1—C8 | 119.17 (16) |
| O1W—Nd1—C8—C7 | −84.3 (10) | O8—Nd1—O1—C8 | −132.82 (14) |
| O2—Nd1—C8—C7 | −83.1 (10) | N1—Nd1—O1—C8 | 64.37 (14) |
| O7—Nd1—C8—C7 | −0.3 (11) | C16—Nd1—O1—C8 | 168.99 (16) |

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| O1—Nd1—C8—C7 | 107.4 (10) | C24—Nd1—O1—C8 | 173.32 (19) |
| O8—Nd1—C8—C7 | −156.8 (9) | O1—C8—O2—Nd1 | −10.8 (2) |
| N1—Nd1—C8—C7 | −5.0 (10) | C7—C8—O2—Nd1 | 167.29 (19) |
| C16—Nd1—C8—C7 | 97.0 (10) | O4—Nd1—O2—C8 | −29.55 (15) |
| C24—Nd1—C8—C7 | −58.0 (12) | O5—Nd1—O2—C8 | 31.64 (16) |
| C14—C9—C10—C11 | 1.2 (4) | O10—Nd1—O2—C8 | 98.31 (14) |
| C15—C9—C10—C11 | −178.8 (3) | O1W—Nd1—O2—C8 | 178.83 (15) |
| C9—C10—C11—C12 | −1.2 (4) | O7—Nd1—O2—C8 | −132.55 (14) |
| C10—C11—C12—O6 | 179.3 (3) | O1—Nd1—O2—C8 | 5.87 (13) |
| C10—C11—C12—C13 | 0.7 (4) | O8—Nd1—O2—C8 | 142.62 (13) |
| C11—C12—C13—C14 | −0.3 (4) | N1—Nd1—O2—C8 | −95.16 (14) |
| O6—C12—C13—C14 | −179.0 (3) | C16—Nd1—O2—C8 | 0.12 (16) |
| C12—C13—C14—C9 | 0.3 (4) | C24—Nd1—O2—C8 | −173.64 (14) |
| C10—C9—C14—C13 | −0.7 (4) | O5—C16—O4—Nd1 | 10.2 (2) |
| C15—C9—C14—C13 | 179.2 (3) | C15—C16—O4—Nd1 | −167.3 (2) |
| C10—C9—C15—C16 | −100.4 (3) | O5—Nd1—O4—C16 | −5.61 (14) |
| C14—C9—C15—C16 | 79.7 (3) | O10—Nd1—O4—C16 | 2.53 (17) |
| C9—C15—C16—O4 | 172.4 (2) | O1W—Nd1—O4—C16 | −144.41 (15) |
| C9—C15—C16—O5 | −5.1 (4) | O2—Nd1—O4—C16 | 107.93 (15) |
| C9—C15—C16—Nd1 | 86.9 (9) | O7—Nd1—O4—C16 | −111.71 (15) |
| O5—Nd1—C16—O4 | 170.0 (2) | O1—Nd1—O4—C16 | 79.82 (15) |
| O10—Nd1—C16—O4 | −177.91 (14) | O8—Nd1—O4—C16 | −67.08 (15) |
| O1W—Nd1—C16—O4 | 97.8 (3) | N1—Nd1—O4—C16 | 171.52 (16) |
| O2—Nd1—C16—O4 | −86.63 (16) | C8—Nd1—O4—C16 | 95.65 (15) |
| O7—Nd1—C16—O4 | 65.29 (15) | C24—Nd1—O4—C16 | −90.75 (15) |
| O1—Nd1—C16—O4 | −91.37 (15) | O4—C16—O5—Nd1 | −10.2 (2) |
| O8—Nd1—C16—O4 | 115.71 (15) | C15—C16—O5—Nd1 | 167.3 (2) |
| N1—Nd1—C16—O4 | −8.47 (16) | O4—Nd1—O5—C16 | 5.57 (14) |
| C8—Nd1—C16—O4 | −86.57 (15) | O10—Nd1—O5—C16 | −167.47 (15) |
| C24—Nd1—C16—O4 | 89.97 (15) | O1W—Nd1—O5—C16 | 151.98 (14) |
| O4—Nd1—C16—O5 | −170.0 (2) | O2—Nd1—O5—C16 | −93.83 (15) |
| O10—Nd1—C16—O5 | 12.10 (15) | O7—Nd1—O5—C16 | 76.08 (14) |
| O1W—Nd1—C16—O5 | −72.2 (3) | O1—Nd1—O5—C16 | −73.46 (14) |
| O2—Nd1—C16—O5 | 103.39 (14) | O8—Nd1—O5—C16 | 123.12 (15) |
| O7—Nd1—C16—O5 | −104.70 (14) | N1—Nd1—O5—C16 | 1.95 (17) |
| O1—Nd1—C16—O5 | 98.64 (15) | C8—Nd1—O5—C16 | −80.52 (15) |
| O8—Nd1—C16—O5 | −54.28 (14) | C24—Nd1—O5—C16 | 99.67 (15) |
| N1—Nd1—C16—O5 | −178.46 (14) | O8—C24—O7—Nd1 | −8.9 (3) |
| C8—Nd1—C16—O5 | 103.44 (14) | C23—C24—O7—Nd1 | 170.0 (2) |
| C24—Nd1—C16—O5 | −80.02 (14) | O4—Nd1—O7—C24 | 121.84 (16) |
| O4—Nd1—C16—C15 | 91.7 (9) | O5—Nd1—O7—C24 | 71.67 (16) |
| O5—Nd1—C16—C15 | −98.3 (9) | O10—Nd1—O7—C24 | −1.60 (17) |
| O10—Nd1—C16—C15 | −86.2 (9) | O1W—Nd1—O7—C24 | −73.62 (16) |
| O1W—Nd1—C16—C15 | −170.5 (8) | O2—Nd1—O7—C24 | −121.51 (15) |
| O2—Nd1—C16—C15 | 5.1 (9) | O1—Nd1—O7—C24 | 143.50 (15) |
| O7—Nd1—C16—C15 | 157.0 (9) | O8—Nd1—O7—C24 | 4.81 (14) |
| O1—Nd1—C16—C15 | 0.3 (9) | N1—Nd1—O7—C24 | −158.61 (17) |
| O8—Nd1—C16—C15 | −152.6 (9) | C16—Nd1—O7—C24 | 97.43 (16) |

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| N1—Nd1—C16—C15 | 83.2 (9) | C8—Nd1—O7—C24 | −163.38 (16) |
| C8—Nd1—C16—C15 | 5.1 (9) | O7—C24—O8—Nd2 | 165.3 (2) |
| C24—Nd1—C16—C15 | −178.3 (9) | C23—C24—O8—Nd2 | −13.7 (5) |
| C22—C17—C18—C19 | 0.1 (4) | Nd1—C24—O8—Nd2 | 156.8 (4) |
| C23—C17—C18—C19 | 178.7 (2) | O7—C24—O8—Nd1 | 8.5 (2) |
| C17—C18—C19—C20 | 0.5 (4) | C23—C24—O8—Nd1 | −170.5 (2) |
| C18—C19—C20—O9 | 179.8 (2) | O14—Nd2—O8—C24 | −82.1 (4) |
| C18—C19—C20—C21 | −1.0 (4) | O13—Nd2—O8—C24 | −74.2 (4) |
| O9—C20—C21—C22 | −179.7 (2) | O2W—Nd2—O8—C24 | 125.5 (4) |
| C19—C20—C21—C22 | 1.1 (4) | O16—Nd2—O8—C24 | 47.9 (4) |
| C20—C21—C22—C17 | −0.5 (4) | O17—Nd2—O8—C24 | −0.6 (4) |
| C18—C17—C22—C21 | 0.0 (4) | O10—Nd2—O8—C24 | −154.7 (4) |
| C23—C17—C22—C21 | −178.6 (2) | O11—Nd2—O8—C24 | −170.0 (3) |
| C18—C17—C23—C24 | −80.7 (3) | N3—Nd2—O8—C24 | 77.0 (4) |
| C22—C17—C23—C24 | 97.9 (3) | C40—Nd2—O8—C24 | −77.4 (4) |
| C17—C23—C24—O7 | −45.7 (4) | C48—Nd2—O8—C24 | 24.6 (4) |
| C17—C23—C24—O8 | 133.3 (3) | C32—Nd2—O8—C24 | −165.1 (4) |
| C17—C23—C24—Nd1 | 29.4 (14) | O14—Nd2—O8—Nd1 | 72.48 (9) |
| O4—Nd1—C24—O7 | −56.16 (16) | O13—Nd2—O8—Nd1 | 80.37 (7) |
| O5—Nd1—C24—O7 | −108.76 (16) | O2W—Nd2—O8—Nd1 | −79.94 (7) |
| O10—Nd1—C24—O7 | 178.57 (16) | O16—Nd2—O8—Nd1 | −157.53 (7) |
| O1W—Nd1—C24—O7 | 99.75 (16) | O17—Nd2—O8—Nd1 | 153.97 (6) |
| O2—Nd1—C24—O7 | 92.10 (19) | O10—Nd2—O8—Nd1 | −0.14 (5) |
| O1—Nd1—C24—O7 | −86.7 (3) | O11—Nd2—O8—Nd1 | −15.42 (8) |
| O8—Nd1—C24—O7 | −171.4 (2) | N3—Nd2—O8—Nd1 | −128.46 (12) |
| N1—Nd1—C24—O7 | 20.79 (16) | C40—Nd2—O8—Nd1 | 77.14 (7) |
| C16—Nd1—C24—O7 | −82.57 (16) | C48—Nd2—O8—Nd1 | 179.17 (7) |
| C8—Nd1—C24—O7 | 72.5 (5) | C32—Nd2—O8—Nd1 | −10.56 (7) |
| O4—Nd1—C24—O8 | 115.28 (14) | O4—Nd1—O8—C24 | −67.55 (14) |
| O5—Nd1—C24—O8 | 62.67 (14) | O5—Nd1—O8—C24 | −113.75 (15) |
| O10—Nd1—C24—O8 | −9.99 (14) | O10—Nd1—O8—C24 | 169.10 (15) |
| O1W—Nd1—C24—O8 | −88.82 (14) | O1W—Nd1—O8—C24 | 83.05 (14) |
| O2—Nd1—C24—O8 | −96.46 (16) | O2—Nd1—O8—C24 | 119.62 (15) |
| O7—Nd1—C24—O8 | 171.4 (2) | O7—Nd1—O8—C24 | −4.66 (14) |
| O1—Nd1—C24—O8 | 84.8 (3) | O1—Nd1—O8—C24 | −144.94 (15) |
| N1—Nd1—C24—O8 | −167.78 (13) | N1—Nd1—O8—C24 | 14.47 (16) |
| C16—Nd1—C24—O8 | 88.87 (14) | C16—Nd1—O8—C24 | −91.73 (15) |
| C8—Nd1—C24—O8 | −116.0 (4) | C8—Nd1—O8—C24 | 161.08 (17) |
| O4—Nd1—C24—C23 | −136.4 (12) | O4—Nd1—O8—Nd2 | 123.50 (7) |
| O5—Nd1—C24—C23 | 171.0 (12) | O5—Nd1—O8—Nd2 | 77.30 (7) |
| O10—Nd1—C24—C23 | 98.4 (12) | O10—Nd1—O8—Nd2 | 0.15 (5) |
| O1W—Nd1—C24—C23 | 19.5 (12) | O1W—Nd1—O8—Nd2 | −85.90 (7) |
| O2—Nd1—C24—C23 | 11.9 (13) | O2—Nd1—O8—Nd2 | −49.33 (11) |
| O7—Nd1—C24—C23 | −80.2 (12) | O7—Nd1—O8—Nd2 | −173.61 (10) |
| O1—Nd1—C24—C23 | −166.9 (11) | O1—Nd1—O8—Nd2 | 46.11 (13) |
| O8—Nd1—C24—C23 | 108.4 (12) | N1—Nd1—O8—Nd2 | −154.48 (7) |
| N1—Nd1—C24—C23 | −59.4 (12) | C16—Nd1—O8—Nd2 | 99.32 (7) |
| C16—Nd1—C24—C23 | −162.8 (12) | C8—Nd1—O8—Nd2 | −7.87 (19) |

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| C8—Nd1—C24—C23 | −7.7 (15) | C24—Nd1—O8—Nd2 | −168.95 (17) |
| C30—C25—C26—C27 | −0.2 (4) | O11—C32—O10—Nd1 | −152.18 (18) |
| C31—C25—C26—C27 | 178.1 (2) | C31—C32—O10—Nd1 | 27.6 (4) |
| C25—C26—C27—C28 | −0.7 (4) | Nd2—C32—O10—Nd1 | −139.3 (2) |
| C26—C27—C28—O12 | −179.1 (2) | O11—C32—O10—Nd2 | −12.9 (2) |
| C26—C27—C28—C29 | 0.9 (4) | C31—C32—O10—Nd2 | 166.9 (2) |
| O12—C28—C29—C30 | 179.8 (2) | O4—Nd1—O10—C32 | 46.8 (3) |
| C27—C28—C29—C30 | −0.1 (4) | O5—Nd1—O10—C32 | 53.6 (2) |
| C26—C25—C30—C29 | 1.0 (4) | O1W—Nd1—O10—C32 | −148.7 (3) |
| C31—C25—C30—C29 | −177.3 (2) | O2—Nd1—O10—C32 | −73.2 (2) |
| C28—C29—C30—C25 | −0.8 (4) | O7—Nd1—O10—C32 | 140.5 (2) |
| C30—C25—C31—C32 | 75.4 (3) | O1—Nd1—O10—C32 | −22.2 (3) |
| C26—C25—C31—C32 | −102.8 (3) | O8—Nd1—O10—C32 | 135.2 (3) |
| C25—C31—C32—O11 | 11.7 (4) | N1—Nd1—O10—C32 | −106.2 (3) |
| C25—C31—C32—O10 | −168.1 (2) | C16—Nd1—O10—C32 | 47.9 (3) |
| C25—C31—C32—Nd2 | −95.1 (8) | C8—Nd1—O10—C32 | −48.0 (3) |
| O8—Nd2—C32—O11 | −169.46 (14) | C24—Nd1—O10—C32 | 139.9 (2) |
| O14—Nd2—C32—O11 | 63.22 (14) | O4—Nd1—O10—Nd2 | −88.51 (8) |
| O13—Nd2—C32—O11 | 115.57 (14) | O5—Nd1—O10—Nd2 | −81.73 (7) |
| O2W—Nd2—C32—O11 | −91.67 (14) | O1W—Nd1—O10—Nd2 | 76.00 (7) |
| O16—Nd2—C32—O11 | −93.24 (16) | O2—Nd1—O10—Nd2 | 151.48 (7) |
| O17—Nd2—C32—O11 | 71.2 (3) | O7—Nd1—O10—Nd2 | 5.24 (9) |
| O10—Nd2—C32—O11 | 167.4 (2) | O1—Nd1—O10—Nd2 | −157.50 (7) |
| N3—Nd2—C32—O11 | −11.06 (15) | O8—Nd1—O10—Nd2 | −0.14 (5) |
| C40—Nd2—C32—O11 | 89.27 (14) | N1—Nd1—O10—Nd2 | 118.49 (13) |
| C48—Nd2—C32—O11 | −64.2 (4) | C16—Nd1—O10—Nd2 | −87.37 (7) |
| O8—Nd2—C32—O10 | 23.18 (14) | C8—Nd1—O10—Nd2 | 176.70 (7) |
| O14—Nd2—C32—O10 | −104.15 (13) | C24—Nd1—O10—Nd2 | 4.57 (7) |
| O13—Nd2—C32—O10 | −51.80 (13) | O8—Nd2—O10—C32 | −154.81 (15) |
| O2W—Nd2—C32—O10 | 100.96 (14) | O14—Nd2—O10—C32 | 74.70 (14) |
| O16—Nd2—C32—O10 | 99.40 (15) | O13—Nd2—O10—C32 | 125.85 (14) |
| O17—Nd2—C32—O10 | −96.2 (2) | O2W—Nd2—O10—C32 | −71.56 (14) |
| O11—Nd2—C32—O10 | −167.4 (2) | O16—Nd2—O10—C32 | −116.31 (14) |
| N3—Nd2—C32—O10 | −178.43 (13) | O17—Nd2—O10—C32 | 141.23 (15) |
| C40—Nd2—C32—O10 | −78.10 (14) | O11—Nd2—O10—C32 | 6.92 (13) |
| C48—Nd2—C32—O10 | 128.5 (4) | N3—Nd2—O10—C32 | 1.90 (15) |
| O8—Nd2—C32—C31 | −56.1 (8) | C40—Nd2—O10—C32 | 99.80 (14) |
| O14—Nd2—C32—C31 | 176.6 (8) | C48—Nd2—O10—C32 | −156.80 (19) |
| O13—Nd2—C32—C31 | −131.1 (8) | O8—Nd2—O10—Nd1 | 0.15 (5) |
| O2W—Nd2—C32—C31 | 21.7 (8) | O14—Nd2—O10—Nd1 | −130.34 (6) |
| O16—Nd2—C32—C31 | 20.1 (8) | O13—Nd2—O10—Nd1 | −79.19 (7) |
| O17—Nd2—C32—C31 | −175.5 (7) | O2W—Nd2—O10—Nd1 | 83.41 (7) |
| O10—Nd2—C32—C31 | −79.3 (8) | O16—Nd2—O10—Nd1 | 38.65 (11) |
| O11—Nd2—C32—C31 | 113.4 (8) | O17—Nd2—O10—Nd1 | −63.81 (14) |
| N3—Nd2—C32—C31 | 102.3 (8) | O11—Nd2—O10—Nd1 | 161.89 (10) |
| C40—Nd2—C32—C31 | −157.4 (8) | N3—Nd2—O10—Nd1 | 156.86 (6) |
| C48—Nd2—C32—C31 | 49.2 (10) | C40—Nd2—O10—Nd1 | −105.23 (7) |
| C38—C33—C34—C35 | −0.8 (4) | C48—Nd2—O10—Nd1 | −1.8 (2) |

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| C39—C33—C34—C35 | 179.0 (2) | C32—Nd2—O10—Nd1 | 154.96 (16) |
| C33—C34—C35—C36 | 0.4 (4) | O10—C32—O11—Nd2 | 12.7 (2) |
| C34—C35—C36—O15 | −179.7 (2) | C31—C32—O11—Nd2 | −167.1 (2) |
| C34—C35—C36—C37 | 0.0 (4) | O8—Nd2—O11—C32 | 11.64 (15) |
| O15—C36—C37—C38 | 179.6 (2) | O14—Nd2—O11—C32 | −112.26 (15) |
| C35—C36—C37—C38 | −0.1 (4) | O13—Nd2—O11—C32 | −66.94 (14) |
| C36—C37—C38—C33 | −0.3 (4) | O2W—Nd2—O11—C32 | 79.80 (14) |
| C34—C33—C38—C37 | 0.8 (4) | O16—Nd2—O11—C32 | 120.02 (14) |
| C39—C33—C38—C37 | −179.1 (2) | O17—Nd2—O11—C32 | −149.58 (14) |
| C38—C33—C39—C40 | −114.6 (3) | O10—Nd2—O11—C32 | −7.00 (13) |
| C34—C33—C39—C40 | 65.6 (3) | N3—Nd2—O11—C32 | 168.79 (15) |
| C33—C39—C40—O14 | 174.1 (2) | C40—Nd2—O11—C32 | −89.67 (14) |
| C33—C39—C40—O13 | −7.1 (3) | C48—Nd2—O11—C32 | 161.92 (16) |
| C33—C39—C40—Nd2 | −127 (4) | O14—C40—O13—Nd2 | 1.4 (2) |
| O8—Nd2—C40—O14 | −171.57 (13) | C39—C40—O13—Nd2 | −177.45 (19) |
| O13—Nd2—C40—O14 | −178.6 (2) | O8—Nd2—O13—C40 | −172.89 (14) |
| O2W—Nd2—C40—O14 | −83.7 (2) | O14—Nd2—O13—C40 | −0.79 (13) |
| O16—Nd2—C40—O14 | 100.30 (15) | O2W—Nd2—O13—C40 | −135.21 (15) |
| O17—Nd2—C40—O14 | 93.01 (14) | O16—Nd2—O13—C40 | 115.13 (14) |
| O10—Nd2—C40—O14 | −106.18 (14) | O17—Nd2—O13—C40 | 84.87 (14) |
| O11—Nd2—C40—O14 | −56.58 (14) | O10—Nd2—O13—C40 | −102.68 (14) |
| N3—Nd2—C40—O14 | 18.80 (15) | O11—Nd2—O13—C40 | −59.81 (14) |
| C48—Nd2—C40—O14 | 94.00 (14) | N3—Nd2—O13—C40 | 21.18 (16) |
| C32—Nd2—C40—O14 | −81.42 (14) | C48—Nd2—O13—C40 | 97.42 (14) |
| O8—Nd2—C40—O13 | 7.00 (14) | C32—Nd2—O13—C40 | −82.53 (14) |
| O14—Nd2—C40—O13 | 178.6 (2) | O13—C40—O14—Nd2 | −1.4 (2) |
| O2W—Nd2—C40—O13 | 94.9 (2) | C39—C40—O14—Nd2 | 177.46 (19) |
| O16—Nd2—C40—O13 | −81.12 (15) | O8—Nd2—O14—C40 | 10.39 (17) |
| O17—Nd2—C40—O13 | −88.42 (14) | O13—Nd2—O14—C40 | 0.80 (13) |
| O10—Nd2—C40—O13 | 72.39 (13) | O2W—Nd2—O14—C40 | 139.55 (14) |
| O11—Nd2—C40—O13 | 122.00 (14) | O16—Nd2—O14—C40 | −99.32 (14) |
| N3—Nd2—C40—O13 | −162.63 (13) | O17—Nd2—O14—C40 | −80.88 (14) |
| C48—Nd2—C40—O13 | −87.43 (14) | O10—Nd2—O14—C40 | 72.34 (14) |
| C32—Nd2—C40—O13 | 97.16 (14) | O11—Nd2—O14—C40 | 119.65 (14) |
| O8—Nd2—C40—C39 | 128 (4) | N3—Nd2—O14—C40 | −160.92 (15) |
| O14—Nd2—C40—C39 | −60 (4) | C48—Nd2—O14—C40 | −91.51 (14) |
| O13—Nd2—C40—C39 | 121 (4) | C32—Nd2—O14—C40 | 96.66 (14) |
| O2W—Nd2—C40—C39 | −144 (4) | O17—C48—O16—Nd2 | 9.9 (2) |
| O16—Nd2—C40—C39 | 40 (4) | C47—C48—O16—Nd2 | −168.96 (19) |
| O17—Nd2—C40—C39 | 33 (4) | O8—Nd2—O16—C48 | −112.64 (14) |
| O10—Nd2—C40—C39 | −166 (4) | O14—Nd2—O16—C48 | 18.09 (16) |
| O11—Nd2—C40—C39 | −117 (4) | O13—Nd2—O16—C48 | −44.57 (15) |
| N3—Nd2—C40—C39 | −42 (4) | O2W—Nd2—O16—C48 | 167.03 (15) |
| C48—Nd2—C40—C39 | 34 (4) | O17—Nd2—O16—C48 | −5.44 (13) |
| C32—Nd2—C40—C39 | −142 (4) | O10—Nd2—O16—C48 | −148.19 (13) |
| C46—C41—C42—C43 | −0.8 (4) | O11—Nd2—O16—C48 | 127.69 (14) |
| C47—C41—C42—C43 | 177.0 (2) | N3—Nd2—O16—C48 | 79.15 (14) |
| C41—C42—C43—C44 | −0.5 (4) | C40—Nd2—O16—C48 | −14.55 (17) |

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| C42—C43—C44—O18 | −178.5 (2) | C32—Nd2—O16—C48 | 168.54 (13) |
| C42—C43—C44—C45 | 1.5 (4) | O16—C48—O17—Nd2 | −9.7 (2) |
| O18—C44—C45—C46 | 178.7 (3) | C47—C48—O17—Nd2 | 169.2 (2) |
| C43—C44—C45—C46 | −1.3 (4) | O8—Nd2—O17—C48 | 78.08 (15) |
| C44—C45—C46—C41 | 0.0 (4) | O14—Nd2—O17—C48 | −155.48 (15) |
| C42—C41—C46—C45 | 1.0 (4) | O13—Nd2—O17—C48 | 150.43 (15) |
| C47—C41—C46—C45 | −176.8 (2) | O2W—Nd2—O17—C48 | −3.80 (17) |
| C46—C41—C47—C48 | 107.6 (3) | O16—Nd2—O17—C48 | 5.36 (13) |
| C42—C41—C47—C48 | −70.1 (3) | O10—Nd2—O17—C48 | 135.10 (14) |
| C41—C47—C48—O16 | 57.1 (3) | O11—Nd2—O17—C48 | −119.06 (15) |
| C41—C47—C48—O17 | −121.8 (3) | N3—Nd2—O17—C48 | −77.75 (15) |
| C41—C47—C48—Nd2 | −23.1 (13) | C40—Nd2—O17—C48 | 177.76 (16) |
| O8—Nd2—C48—O16 | 66.10 (14) | C32—Nd2—O17—C48 | −163.57 (18) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3*B*···O12$^{i}$ | 0.82 | 1.94 | 2.751 (3) | 170 |
| O6—H6*B*···O3*W*$^{ii}$ | 0.82 | 1.86 | 2.647 (3) | 160 |
| O9—H9*A*···O17$^{iii}$ | 0.82 | 1.86 | 2.676 (3) | 173 |
| O12—H12*A*···O11$^{iv}$ | 0.82 | 1.94 | 2.746 (2) | 167 |
| O15—H15*C*···O6$^{v}$ | 0.82 | 1.91 | 2.725 (3) | 173 |
| O18—H18*B*···O9$^{ii}$ | 0.82 | 1.95 | 2.763 (3) | 173 |
| O2*W*—H2*WA*···O5 | 0.82 (2) | 2.02 (2) | 2.772 (2) | 153 (3) |
| O2*W*—H2*WB*···N2$^{ii}$ | 0.81 (2) | 2.04 (2) | 2.840 (3) | 170 (3) |
| O3*W*—H3*WB*···O3 | 0.82 (2) | 2.02 (2) | 2.811 (3) | 162 (3) |
| O1*W*—H1*WA*···O13 | 0.81 (2) | 1.98 (2) | 2.764 (2) | 161 (3) |
| O1*W*—H1*WB*···N4$^{i}$ | 0.82 (2) | 1.99 (2) | 2.775 (3) | 161 (3) |
| O3*W*—H3*WA*···O1$^{vi}$ | 0.82 (2) | 1.95 (2) | 2.770 (3) | 175 (4) |
| C6—H6*A*···O2$^{vii}$ | 0.93 | 2.49 | 3.283 (3) | 144 |
| C31—H31*A*···O1 | 0.97 | 2.58 | 3.338 (3) | 135 |
| C49—H49*A*···O2 | 0.93 | 2.42 | 3.038 (3) | 124 |
| C59—H59*A*···O16 | 0.93 | 2.57 | 3.191 (3) | 125 |
| C63—H63*A*···O14 | 0.93 | 2.45 | 3.095 (3) | 126 |

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*, *y*−1, *z*; (iii) −*x*, −*y*+1, −*z*; (iv) −*x*, −*y*, −*z*+1; (v) *x*−1, *y*+1, *z*; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) −*x*, −*y*+1, −*z*+1.