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# *catena*-Poly[[penta-$\mu$-benzoato-$\mu$-chlorido-dioxanedineodymium(III)] dioxane 2.5-solvate]

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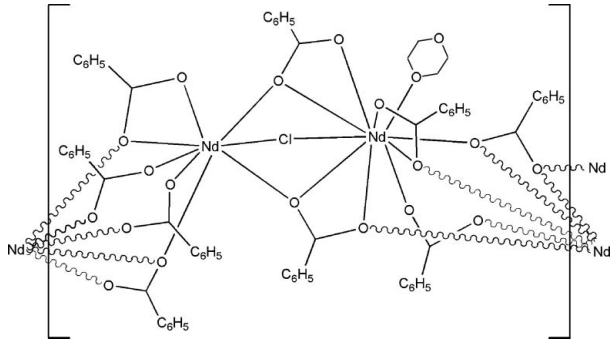
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.015 Å; some non-H atoms missing; disorder in main residue; $R$ factor = 0.052; $wR$ factor = 0.119; data-to-parameter ratio = 19.0.

The asymmetric unit of the title compound, $[Nd_2(C_6H_5COO)_5Cl(C_4H_8O_2)]\cdot 2.5C_4H_8O_2$, consists of two $Nd^{III}$ ions bridged by one $Cl^-$ ion, five benzoate ions and one coordinating 1,4-dioxane molecule. One $Nd^{III}$ ion is nine-coordinate, with a very distorted monocapped square-antiprismatic geometry. It is coordinated by two chelating carboxylate groups, three monodentate carboxylate groups, one chloride ion and one dioxane molecule. A second independent $Nd^{III}$ ion is eight-coordinated in a distorted square-antiprismatic geometry by one chelating carboxylate group, five monodentate carboxylate groups and one chloride ion. The chains of the extended structure are parallel to the crystallographic $b$ axis. There is a small amount of void space which is filled with five disordered dioxane solvent molecules per unit cell. The intensity contribution of the disordered solvent molecules was removed by applying the *SQUEEZE* procedure in *PLATON* [Spek (2009). *Acta Cryst.* D**65**, 148–155].

## Related literature

For recent research on ditopic-linked secondary building units, see: Morris *et al.* (2008). For 2-D neodymium adducts, see: Nayak *et al.* (2010). For the synthesis of the neodymium precursor, see: Andersen *et al.* (1978). For SQUEEZE analysis of the data, see: Spek (2009).




## Experimental

### Crystal data

$[Nd_2(C_7H_5O_2)_5Cl(C_4H_8O_2)]\cdot 2.5C_4H_8O_2$
$M_r$ = 1237.84
Triclinic, $P\overline{1}$
$a$ = 12.7631 (5) Å
$b$ = 13.6077 (6) Å
$c$ = 14.2614 (7) Å
$\alpha$ = 102.785 (3)°
$\beta$ = 96.943 (3)°
$\gamma$ = 104.316 (3)°
$V$ = 2299.68 (18) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 2.37 mm$^{-1}$
$T$ = 100 K
0.32 × 0.18 × 0.16 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
$T_{min}$ = 0.606, $T_{max}$ = 0.685
27066 measured reflections
8104 independent reflections
4870 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.087

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.119
$S$ = 0.90
8104 reflections
427 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.45 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.94 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008; 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: *SHELXTL* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2541).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, m690 [doi:10.1107/S1600536812017746]

## *catena*-Poly[[penta-$\mu$-benzoato-$\mu$-chlorido-dioxanedineodymium(III)] dioxane 2.5-solvate]

**Jeffrey A. Bertke, Allen G. Oliver and Kenneth W. Henderson**

### Comment

We are interested in building three-dimensional materials using pre-assembled molecular aggregates as secondary building units (SBUs) linked through ditopic organic molecules (Morris *et al.*, 2008). The title compound was synthesized with this goal in mind. However, instead of forming neodymium-benzoate SBUs which could be linked through 1,4-dioxane, a 1-D neodymium-benzoate polymer was crystallized. The closely related compound $[Nd_2(C_6H_5COO)_6(CH_3OH)_4]$ was previously reported as a 2-D material from PXRD data(Nayak *et al.*, 2010).

The asymmetric unit consists of two $Nd^{3+}$ metal centers bridged by one $Cl^-$ ion, five benzoate ions and one coordinated 1,4-dioxane molecule (Figure 1). The presence of chloride can be explained as carry-over from the synthesis of $Nd(O^iPr)_3$ which is synthesized from $NdCl_3$ and $NaO^iPr$ (Andersen *et al.*, 1978). The extended crystal structure is a 1-D polymeric chain composed of Nd/Cl/carboxylate interactions. The dioxane solvent molecule acts as a terminal donor. The 1-D chains extend along the crystallographic *b*-axis (Figure 2). Small channels also run along the crystallographic *b*-axis and are filled with disordered solvent molecules. The solvent could not be reliably modeled and was omitted through use of the SQUEEZE routine within *PLATON* (Spek, 2009; see refinement procedures for details).

Nd1 adopts a 9-coordinate distorted mono-capped square anti-prismatic geometry. It is coordinated by two chelating carboxylate groups, three monodentate carboxylate groups, one bridging chloride ion and one terminally coordinating dioxane molecule. Nd2 is 8-coordinate in a distorted square anti-prismatic geometry. It is coordinated by one chelating carboxylate group, five monodentate carboxylate groups and the bridging chloride ion.

### Experimental

Benzoic acid was purchased from Aldrich and used without further purification. $Nd(OiPr)_3$ was purchased from Strem and used without further purification. 1,4-dioxane was distilled onto molecular sieves from potassium benzophenone.

Benzoic acid (0.366 g, 3 mmol) was dissolved in 1,4-dioxane (20 ml). Solid $Nd(O^iPr)_3$ (0.321 g, 1 mmol) was added and the solution was refluxed overnight. The solution was allowed to cool to room temperature and then filtered. The filtrate was concentrated and single crystals were grown upon cooling of this saturated solution to room temperature in a hot water bath over the course of several days. Crystalline yield 0.069 g (11.14%) calculated based on Nd.

### Refinement

Hydrogen atoms were included in idealized geometries riding on the atom to which they are bonded. Aromatic C–H distances were constrained to 0.95 Å and methylene C–H distances constrained to 0.99 Å. All hydrogen thermal parameters were set to 1.2 × $U_{eq}$ of the carbon to which they are bonded.

Disordered solvent could not be reliably modeled and was thus omitted from the model through the use of SQUEEZE (Spek, 2009). The void space analysis yielded a volume of 540 Å$^3$ with an electron count of 224, located at a center of

symmetry. This corresponds well to five molecules of dioxane per unit cell. The atom count has been corrected to reflect this solvent inclusion.

### Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008; data reduction: *SAINT* (Bruker, 2008; 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: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

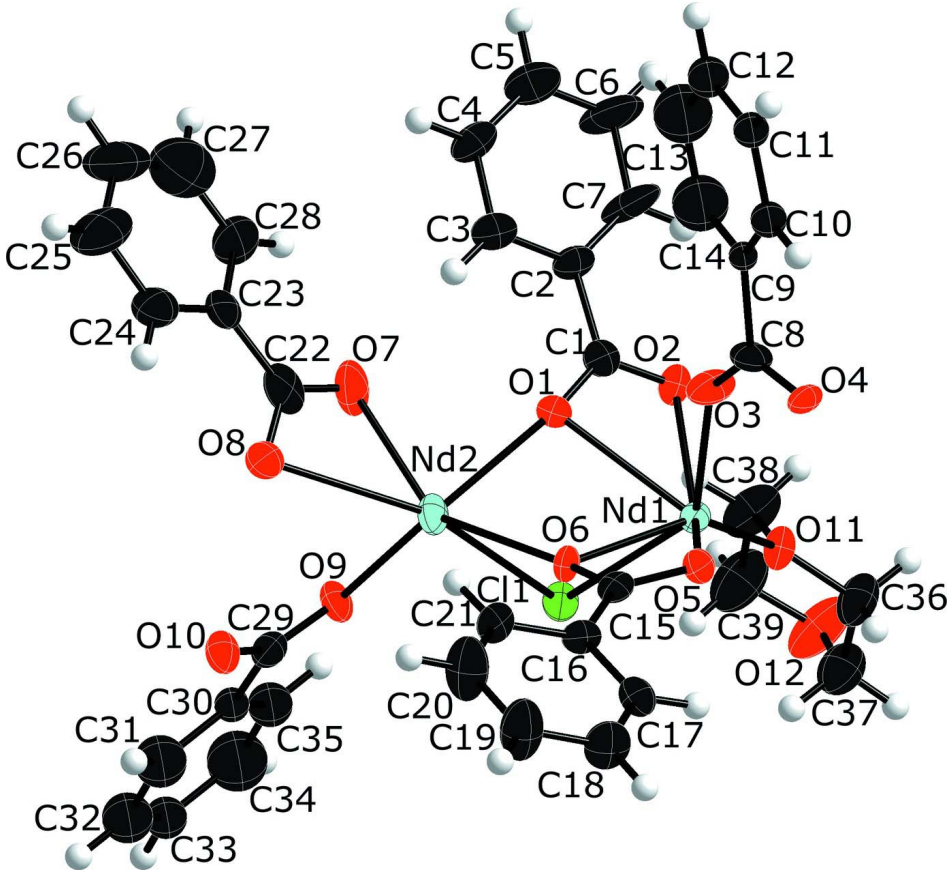


**Figure 1**

Labelling scheme for I. Thermal ellipsoids represented at 50% probability. H atoms depicted as spheres of a fixed radius.

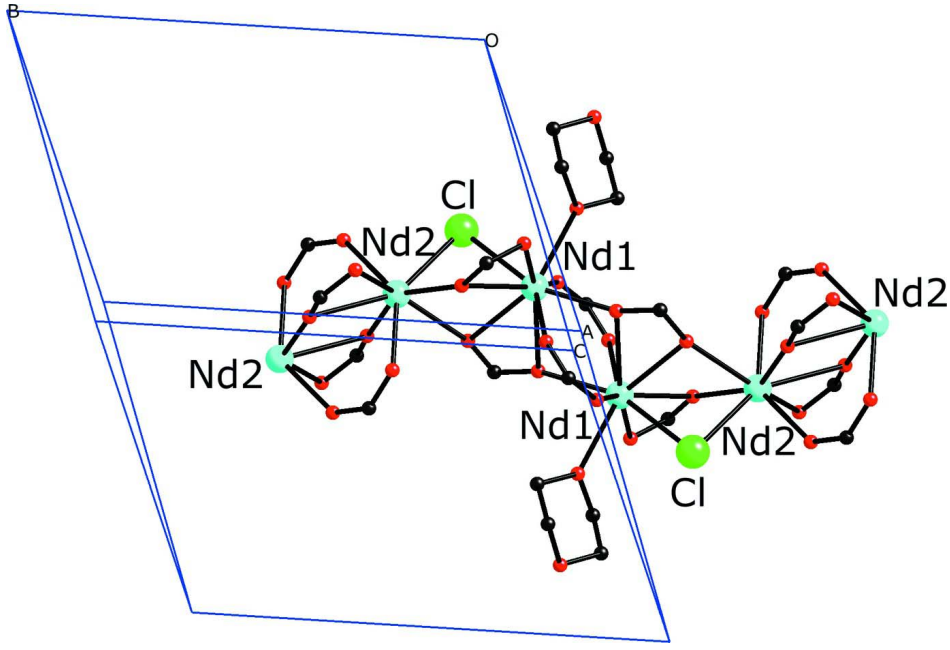


**Figure 2**

Extended structure, with the one-dimensional chain extending along the *b*-axis. All phenyl rings of the benzoate ligands and all hydrogen atoms have been removed for clarity.

**_catena_-Poly[[penta-$\mu$-benzoato-$\mu$-chlorido-dioxanedineodymium(III)] dioxane 2.5-solvate]**

*Crystal data*

$[Nd_2(C_7H_5O_2)_5Cl(C_4H_8O_2)]\cdot 2.5C_4H_8O_2$
$M_r$ = 1237.84
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 12.7631 (5) Å
$b$ = 13.6077 (6) Å
$c$ = 14.2614 (7) Å
$\alpha$ = 102.785 (3)°
$\beta$ = 96.943 (3)°
$\gamma$ = 104.316 (3)°
$V$ = 2299.68 (18) Å$^3$
$Z$ = 2
$F(000)$ = 1240
$D_x$ = 1.788 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2312 reflections
$\theta$ = 2.4–19.0°
$\mu$ = 2.37 mm$^{-1}$
$T$ = 100 K
Needle, blue
0.32 × 0.18 × 0.16 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
$T_{min}$ = 0.606, $T_{max}$ = 0.685
27066 measured reflections
8104 independent reflections
4870 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.087
$\theta_{max}$ = 25.1°, $\theta_{min}$ = 1.5°
$h$ = −15→15
$k$ = −16→16
$l$ = −13→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.119$
$S = 0.90$
8104 reflections
427 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.45$ e Å$^{-3}$
$\Delta\rho_{min} = -0.94$ e Å$^{-3}$

*Special details*

**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.

**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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Nd1 | 0.42843 (3) | 0.05580 (3) | 0.39858 (3) | 0.02441 (14) | |
| Nd2 | 0.46041 (4) | 0.35430 (3) | 0.41815 (4) | 0.03265 (16) | |
| Cl1 | 0.27807 (15) | 0.17311 (16) | 0.36816 (16) | 0.0329 (5) | |
| O1 | 0.5172 (4) | 0.2130 (4) | 0.3257 (4) | 0.0310 (14) | |
| O2 | 0.4585 (4) | 0.0526 (4) | 0.2303 (4) | 0.0341 (14) | |
| O3 | 0.6189 (4) | 0.0707 (5) | 0.3970 (5) | 0.0456 (17) | |
| O4 | 0.7013 (4) | 0.0001 (4) | 0.5011 (4) | 0.0316 (14) | |
| O5 | 0.4679 (4) | −0.1024 (4) | 0.4236 (4) | 0.0300 (13) | |
| O6 | 0.5077 (4) | −0.2327 (4) | 0.4716 (4) | 0.0291 (13) | |
| O7 | 0.5231 (7) | 0.4308 (5) | 0.2902 (5) | 0.063 (2) | |
| O8 | 0.5524 (4) | 0.5571 (4) | 0.4251 (4) | 0.0368 (15) | |
| O9 | 0.3103 (4) | 0.4307 (4) | 0.3939 (4) | 0.0358 (15) | |
| O10 | 0.3508 (4) | 0.5843 (4) | 0.5070 (4) | 0.0377 (15) | |
| O11 | 0.2669 (4) | −0.0860 (4) | 0.2839 (4) | 0.0374 (15) | |
| O12 | 0.0494 (6) | −0.1857 (6) | 0.1846 (5) | 0.074 (2) | |
| C1 | 0.5171 (7) | 0.1464 (7) | 0.2475 (6) | 0.032 (2) | |
| C2 | 0.5931 (7) | 0.1778 (7) | 0.1806 (6) | 0.034 (2) | |
| C3 | 0.6589 (7) | 0.2799 (7) | 0.1979 (7) | 0.041 (2) | |
| H3 | 0.6534 | 0.3332 | 0.2512 | 0.049* | |
| C4 | 0.7321 (7) | 0.3036 (8) | 0.1375 (7) | 0.044 (2) | |
| H4 | 0.7758 | 0.3739 | 0.1480 | 0.052* | |
| C5 | 0.7424 (9) | 0.2266 (9) | 0.0625 (8) | 0.061 (3) | |
| H5 | 0.7949 | 0.2431 | 0.0224 | 0.074* | |
| C6 | 0.6765 (11) | 0.1250 (10) | 0.0450 (9) | 0.087 (4) | |
| H6 | 0.6828 | 0.0715 | −0.0077 | 0.104* | |
| C7 | 0.6023 (9) | 0.1019 (8) | 0.1038 (7) | 0.062 (3) | |

| | | | | | |
|---|---|---|---|---|---|
| H7 | 0.5563 | 0.0321 | 0.0913 | 0.074* | |
| C8 | 0.7002 (7) | 0.0470 (7) | 0.4349 (7) | 0.036 (2) | |
| C15 | 0.4761 (6) | −0.1963 (6) | 0.4033 (6) | 0.0265 (19) | |
| C16 | 0.4459 (6) | −0.2587 (7) | 0.2995 (6) | 0.029 (2) | |
| C17 | 0.4655 (7) | −0.2070 (7) | 0.2282 (6) | 0.036 (2) | |
| H17 | 0.4979 | −0.1331 | 0.2458 | 0.043* | |
| C18 | 0.4375 (8) | −0.2634 (8) | 0.1285 (7) | 0.049 (3) | |
| H18 | 0.4518 | −0.2286 | 0.0786 | 0.059* | |
| C19 | 0.3889 (10) | −0.3704 (8) | 0.1055 (8) | 0.066 (3) | |
| H19 | 0.3696 | −0.4097 | 0.0389 | 0.079* | |
| C20 | 0.3682 (9) | −0.4208 (8) | 0.1774 (7) | 0.063 (3) | |
| H20 | 0.3328 | −0.4941 | 0.1598 | 0.075* | |
| C21 | 0.3980 (6) | −0.3665 (6) | 0.2748 (6) | 0.033 (2) | |
| H21 | 0.3859 | −0.4023 | 0.3243 | 0.039* | |
| C22 | 0.5731 (9) | 0.5236 (9) | 0.3398 (8) | 0.052 (3) | |
| C23 | 0.6533 (9) | 0.5968 (8) | 0.3005 (8) | 0.050 (3) | |
| C24 | 0.7152 (8) | 0.6935 (8) | 0.3578 (8) | 0.053 (3) | |
| H24 | 0.7077 | 0.7161 | 0.4240 | 0.063* | |
| C25 | 0.7892 (9) | 0.7580 (11) | 0.3175 (11) | 0.080 (4) | |
| H25 | 0.8355 | 0.8241 | 0.3564 | 0.096* | |
| C26 | 0.7940 (11) | 0.7236 (13) | 0.2186 (12) | 0.091 (5) | |
| H26 | 0.8449 | 0.7665 | 0.1905 | 0.110* | |
| C27 | 0.7268 (14) | 0.6292 (14) | 0.1617 (11) | 0.099 (5) | |
| H27 | 0.7296 | 0.6084 | 0.0941 | 0.119* | |
| C28 | 0.6564 (11) | 0.5655 (10) | 0.2008 (9) | 0.076 (4) | |
| H28 | 0.6096 | 0.5000 | 0.1612 | 0.092* | |
| C29 | 0.2858 (7) | 0.5090 (7) | 0.4387 (7) | 0.034 (2) | |
| C36 | 0.2039 (7) | −0.1803 (7) | 0.3002 (8) | 0.056 (3) | |
| H36A | 0.2273 | −0.1824 | 0.3683 | 0.067* | |
| H36B | 0.2163 | −0.2415 | 0.2555 | 0.067* | |
| C37 | 0.0851 (8) | −0.1856 (8) | 0.2826 (8) | 0.060 (3) | |
| H37A | 0.0415 | −0.2503 | 0.2961 | 0.072* | |
| H37B | 0.0729 | −0.1245 | 0.3277 | 0.072* | |
| C38 | 0.2271 (8) | −0.0800 (8) | 0.1877 (7) | 0.060 (3) | |
| H38A | 0.2405 | −0.1372 | 0.1386 | 0.072* | |
| H38B | 0.2679 | −0.0122 | 0.1778 | 0.072* | |
| C39 | 0.1106 (9) | −0.0887 (10) | 0.1734 (9) | 0.078 (4) | |
| H39A | 0.0973 | −0.0306 | 0.2216 | 0.093* | |
| H39B | 0.0858 | −0.0825 | 0.1071 | 0.093* | |
| C9 | 0.8010 (9) | 0.0640 (11) | 0.3862 (10) | 0.021 (4)* | 0.50 |
| C10 | 0.9017 (11) | 0.0620 (12) | 0.4340 (9) | 0.032 (9)* | 0.50 |
| H10 | 0.9062 | 0.0414 | 0.4935 | 0.038* | 0.50 |
| C11 | 0.9959 (8) | 0.0900 (11) | 0.3948 (10) | 0.031 (6)* | 0.50 |
| H11 | 1.0647 | 0.0886 | 0.4275 | 0.037* | 0.50 |
| C12 | 0.9893 (9) | 0.1201 (10) | 0.3077 (10) | 0.041 (5)* | 0.50 |
| H12 | 1.0537 | 0.1392 | 0.2810 | 0.049* | 0.50 |
| C13 | 0.8886 (11) | 0.1221 (12) | 0.2599 (8) | 0.084 (8)* | 0.50 |
| H13 | 0.8842 | 0.1426 | 0.2004 | 0.101* | 0.50 |
| C14 | 0.7945 (9) | 0.0941 (12) | 0.2991 (10) | 0.076 (7)* | 0.50 |

| | | | | | |
|---|---|---|---|---|---|
| H14 | 0.7257 | 0.0955 | 0.2664 | 0.092* | 0.50 |
| C9A | 0.8092 (8) | 0.0957 (9) | 0.4084 (8) | 0.019 (4)* | 0.50 |
| C10A | 0.9047 (11) | 0.0748 (11) | 0.4459 (9) | 0.040 (10)* | 0.50 |
| H10A | 0.9030 | 0.0344 | 0.4925 | 0.048* | 0.50 |
| C11A | 1.0026 (8) | 0.1131 (11) | 0.4154 (10) | 0.032 (6)* | 0.50 |
| H11A | 1.0678 | 0.0988 | 0.4411 | 0.039* | 0.50 |
| C12A | 1.0050 (7) | 0.1723 (9) | 0.3474 (9) | 0.037 (4)* | 0.50 |
| H12A | 1.0720 | 0.1984 | 0.3265 | 0.044* | 0.50 |
| C13A | 0.9096 (8) | 0.1931 (8) | 0.3098 (8) | 0.042 (5)* | 0.50 |
| H13A | 0.9113 | 0.2336 | 0.2633 | 0.051* | 0.50 |
| C14A | 0.8117 (7) | 0.1548 (8) | 0.3403 (8) | 0.022 (3)* | 0.50 |
| H14A | 0.7465 | 0.1691 | 0.3147 | 0.026* | 0.50 |
| C30 | 0.1778 (10) | 0.5269 (13) | 0.4109 (13) | 0.029 (7)* | 0.50 |
| C31 | 0.1526 (13) | 0.6120 (13) | 0.4677 (12) | 0.066 (10)* | 0.50 |
| H31 | 0.2060 | 0.6599 | 0.5210 | 0.079* | 0.50 |
| C32 | 0.0493 (14) | 0.6268 (12) | 0.4467 (12) | 0.062 (8)* | 0.50 |
| H32 | 0.0321 | 0.6850 | 0.4856 | 0.074* | 0.50 |
| C33 | −0.0288 (10) | 0.5566 (13) | 0.3688 (11) | 0.043 (5)* | 0.50 |
| H33 | −0.0994 | 0.5668 | 0.3544 | 0.052* | 0.50 |
| C34 | −0.0036 (11) | 0.4716 (11) | 0.3119 (10) | 0.089 (8)* | 0.50 |
| H34 | −0.0570 | 0.4236 | 0.2587 | 0.106* | 0.50 |
| C35 | 0.0997 (12) | 0.4567 (10) | 0.3329 (10) | 0.048 (5)* | 0.50 |
| H35 | 0.1169 | 0.3986 | 0.2941 | 0.058* | 0.50 |
| C30A | 0.1673 (10) | 0.5126 (12) | 0.4180 (12) | 0.031 (7)* | 0.50 |
| C31A | 0.1370 (11) | 0.6039 (10) | 0.4499 (13) | 0.032 (6)* | 0.50 |
| H31A | 0.1903 | 0.6658 | 0.4894 | 0.039* | 0.50 |
| C32A | 0.0287 (12) | 0.6048 (11) | 0.4242 (13) | 0.035 (5)* | 0.50 |
| H32A | 0.0080 | 0.6673 | 0.4460 | 0.043* | 0.50 |
| C33A | −0.0493 (9) | 0.5143 (14) | 0.3665 (12) | 0.079 (9)* | 0.50 |
| H33A | −0.1233 | 0.5149 | 0.3489 | 0.095* | 0.50 |
| C34A | −0.0190 (12) | 0.4229 (11) | 0.3346 (11) | 0.098 (9)* | 0.50 |
| H34A | −0.0723 | 0.3611 | 0.2951 | 0.117* | 0.50 |
| C35A | 0.0892 (13) | 0.4221 (10) | 0.3603 (11) | 0.055 (6)* | 0.50 |
| H35A | 0.1099 | 0.3596 | 0.3385 | 0.066* | 0.50 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Nd1 | 0.0195 (2) | 0.0248 (3) | 0.0326 (3) | 0.00797 (19) | 0.0064 (2) | 0.0122 (2) |
| Nd2 | 0.0263 (3) | 0.0245 (3) | 0.0492 (4) | 0.0104 (2) | 0.0034 (2) | 0.0121 (2) |
| Cl1 | 0.0200 (10) | 0.0315 (11) | 0.0472 (14) | 0.0080 (8) | 0.0016 (9) | 0.0118 (10) |
| O1 | 0.032 (3) | 0.030 (3) | 0.033 (4) | 0.010 (3) | 0.011 (3) | 0.008 (3) |
| O2 | 0.034 (3) | 0.027 (3) | 0.039 (4) | 0.003 (3) | 0.004 (3) | 0.011 (3) |
| O3 | 0.020 (3) | 0.069 (4) | 0.064 (4) | 0.019 (3) | 0.015 (3) | 0.040 (4) |
| O4 | 0.025 (3) | 0.042 (3) | 0.044 (4) | 0.015 (3) | 0.017 (3) | 0.031 (3) |
| O5 | 0.031 (3) | 0.027 (3) | 0.036 (4) | 0.012 (2) | 0.008 (3) | 0.011 (3) |
| O6 | 0.030 (3) | 0.028 (3) | 0.037 (4) | 0.012 (2) | 0.007 (3) | 0.018 (3) |
| O7 | 0.118 (7) | 0.041 (4) | 0.048 (5) | 0.040 (4) | 0.026 (4) | 0.021 (4) |
| O8 | 0.033 (3) | 0.040 (4) | 0.044 (4) | 0.016 (3) | 0.009 (3) | 0.015 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O9 | 0.028 (3) | 0.027 (3) | 0.051 (4) | 0.013 (3) | 0.004 (3) | 0.005 (3) |
| O10 | 0.027 (3) | 0.029 (3) | 0.055 (4) | 0.009 (3) | 0.002 (3) | 0.009 (3) |
| O11 | 0.038 (3) | 0.028 (3) | 0.044 (4) | 0.003 (3) | 0.004 (3) | 0.014 (3) |
| O12 | 0.048 (4) | 0.090 (6) | 0.059 (5) | −0.025 (4) | −0.019 (4) | 0.034 (4) |
| C1 | 0.027 (5) | 0.038 (5) | 0.036 (6) | 0.017 (4) | 0.003 (4) | 0.017 (5) |
| C2 | 0.032 (5) | 0.048 (6) | 0.028 (5) | 0.013 (4) | 0.008 (4) | 0.022 (5) |
| C3 | 0.034 (5) | 0.052 (6) | 0.039 (6) | 0.009 (4) | 0.008 (4) | 0.017 (5) |
| C4 | 0.031 (5) | 0.048 (6) | 0.049 (7) | −0.002 (4) | 0.004 (5) | 0.024 (5) |
| C5 | 0.067 (8) | 0.079 (8) | 0.043 (7) | 0.016 (6) | 0.021 (6) | 0.027 (6) |
| C6 | 0.112 (11) | 0.074 (9) | 0.062 (8) | −0.009 (8) | 0.059 (8) | 0.010 (7) |
| C7 | 0.072 (8) | 0.057 (7) | 0.042 (7) | −0.017 (6) | 0.027 (6) | 0.012 (6) |
| C8 | 0.023 (5) | 0.044 (5) | 0.044 (6) | 0.012 (4) | 0.014 (4) | 0.010 (5) |
| C15 | 0.012 (4) | 0.032 (5) | 0.034 (5) | 0.002 (3) | 0.002 (4) | 0.011 (4) |
| C16 | 0.023 (4) | 0.043 (5) | 0.027 (5) | 0.009 (4) | 0.001 (4) | 0.022 (4) |
| C17 | 0.034 (5) | 0.035 (5) | 0.039 (6) | 0.015 (4) | 0.005 (4) | 0.007 (5) |
| C18 | 0.064 (7) | 0.055 (7) | 0.029 (6) | 0.016 (5) | 0.003 (5) | 0.016 (5) |
| C19 | 0.101 (9) | 0.046 (7) | 0.045 (7) | 0.016 (6) | 0.000 (6) | 0.012 (6) |
| C20 | 0.090 (9) | 0.042 (6) | 0.043 (7) | 0.014 (6) | −0.013 (6) | 0.003 (6) |
| C21 | 0.034 (5) | 0.038 (5) | 0.036 (6) | 0.016 (4) | 0.001 (4) | 0.024 (4) |
| C22 | 0.076 (8) | 0.059 (7) | 0.044 (7) | 0.050 (6) | 0.010 (6) | 0.029 (6) |
| C23 | 0.068 (7) | 0.047 (6) | 0.062 (8) | 0.041 (6) | 0.036 (6) | 0.031 (6) |
| C24 | 0.046 (6) | 0.065 (7) | 0.063 (7) | 0.027 (6) | 0.023 (6) | 0.029 (6) |
| C25 | 0.039 (7) | 0.100 (10) | 0.115 (12) | 0.012 (6) | 0.025 (7) | 0.058 (9) |
| C26 | 0.071 (9) | 0.129 (14) | 0.108 (13) | 0.031 (9) | 0.054 (9) | 0.076 (11) |
| C27 | 0.119 (14) | 0.124 (14) | 0.081 (11) | 0.062 (12) | 0.031 (10) | 0.042 (11) |
| C28 | 0.127 (12) | 0.064 (8) | 0.063 (9) | 0.040 (8) | 0.053 (8) | 0.036 (7) |
| C29 | 0.027 (5) | 0.036 (5) | 0.049 (6) | 0.013 (4) | 0.010 (4) | 0.023 (5) |
| C36 | 0.043 (6) | 0.041 (6) | 0.081 (8) | 0.002 (5) | 0.002 (5) | 0.026 (6) |
| C37 | 0.050 (7) | 0.054 (7) | 0.073 (8) | 0.004 (5) | 0.005 (6) | 0.024 (6) |
| C38 | 0.058 (7) | 0.069 (7) | 0.045 (7) | −0.002 (6) | −0.010 (5) | 0.031 (6) |
| C39 | 0.056 (7) | 0.083 (9) | 0.085 (9) | −0.003 (6) | −0.008 (6) | 0.040 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Nd1—O3 | 2.392 (5) | C22—C23 | 1.495 (14) |
| Nd1—O4$^{i}$ | 2.409 (5) | C23—C24 | 1.370 (13) |
| Nd1—O5 | 2.418 (5) | C23—C28 | 1.399 (14) |
| Nd1—O2 | 2.469 (5) | C24—C25 | 1.392 (14) |
| Nd1—O11 | 2.543 (5) | C24—H24 | 0.9500 |
| Nd1—O6$^{i}$ | 2.565 (5) | C25—C26 | 1.398 (17) |
| Nd1—O5$^{i}$ | 2.578 (5) | C25—H25 | 0.9500 |
| Nd1—O1 | 2.647 (5) | C26—C27 | 1.368 (18) |
| Nd1—Cl1 | 2.835 (2) | C26—H26 | 0.9500 |
| Nd1—C1 | 2.918 (9) | C27—C28 | 1.349 (17) |
| Nd1—C15$^{i}$ | 2.958 (8) | C27—H27 | 0.9500 |
| Nd1—Nd2 | 3.9235 (6) | C28—H28 | 0.9500 |
| Nd2—O8$^{ii}$ | 2.339 (6) | C29—C30 | 1.482 (13) |
| Nd2—O10$^{ii}$ | 2.373 (5) | C29—C30A | 1.521 (13) |
| Nd2—O1 | 2.400 (5) | C36—C37 | 1.488 (13) |
| Nd2—O7 | 2.415 (7) | C36—H36A | 0.9900 |

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|---|---|---|---|
| Nd2—O9 | 2.420 (5) | C36—H36B | 0.9900 |
| Nd2—O6$^{i}$ | 2.589 (5) | C37—H37A | 0.9900 |
| Nd2—O8 | 2.693 (6) | C37—H37B | 0.9900 |
| Nd2—Cl1 | 2.826 (2) | C38—C39 | 1.447 (14) |
| Nd2—C22 | 2.918 (11) | C38—H38A | 0.9900 |
| Nd2—Nd2$^{ii}$ | 3.9428 (9) | C38—H38B | 0.9900 |
| O1—C1 | 1.272 (9) | C39—H39A | 0.9900 |
| O2—C1 | 1.262 (9) | C39—H39B | 0.9900 |
| O3—C8 | 1.258 (10) | C9—C10 | 1.3900 |
| O4—C8 | 1.251 (10) | C9—C14 | 1.3900 |
| O4—Nd1$^{i}$ | 2.409 (5) | C10—C11 | 1.3900 |
| O5—C15 | 1.280 (9) | C10—H10 | 0.9500 |
| O5—Nd1$^{i}$ | 2.578 (5) | C11—C12 | 1.3900 |
| O6—C15 | 1.254 (9) | C11—H11 | 0.9500 |
| O6—Nd1$^{i}$ | 2.565 (5) | C12—C13 | 1.3900 |
| O6—Nd2$^{i}$ | 2.589 (5) | C12—H12 | 0.9500 |
| O7—C22 | 1.265 (12) | C13—C14 | 1.3900 |
| O8—C22 | 1.284 (11) | C13—H13 | 0.9500 |
| O8—Nd2$^{ii}$ | 2.339 (6) | C14—H14 | 0.9500 |
| O9—C29 | 1.246 (9) | C9A—C10A | 1.3900 |
| O10—C29 | 1.276 (10) | C9A—C14A | 1.3900 |
| O10—Nd2$^{ii}$ | 2.373 (5) | C10A—C11A | 1.3900 |
| O11—C36 | 1.419 (10) | C10A—H10A | 0.9500 |
| O11—C38 | 1.431 (10) | C11A—C12A | 1.3900 |
| O12—C39 | 1.411 (12) | C11A—H11A | 0.9500 |
| O12—C37 | 1.417 (11) | C12A—C13A | 1.3900 |
| C1—C2 | 1.495 (11) | C12A—H12A | 0.9500 |
| C2—C7 | 1.368 (12) | C13A—C14A | 1.3900 |
| C2—C3 | 1.384 (12) | C13A—H13A | 0.9500 |
| C3—C4 | 1.374 (12) | C14A—H14A | 0.9500 |
| C3—H3 | 0.9500 | C30—C31 | 1.3900 |
| C4—C5 | 1.365 (13) | C30—C35 | 1.3900 |
| C4—H4 | 0.9500 | C31—C32 | 1.3900 |
| C5—C6 | 1.379 (15) | C31—H31 | 0.9500 |
| C5—H5 | 0.9500 | C32—C33 | 1.3900 |
| C6—C7 | 1.366 (13) | C32—H32 | 0.9500 |
| C6—H6 | 0.9500 | C33—C34 | 1.3900 |
| C7—H7 | 0.9500 | C33—H33 | 0.9500 |
| C8—C9A | 1.517 (12) | C34—C35 | 1.3900 |
| C8—C9 | 1.528 (12) | C34—H34 | 0.9500 |
| C15—C16 | 1.486 (11) | C35—H35 | 0.9500 |
| C15—Nd1$^{i}$ | 2.958 (8) | C30A—C31A | 1.3900 |
| C16—C17 | 1.373 (11) | C30A—C35A | 1.3900 |
| C16—C21 | 1.387 (11) | C31A—C32A | 1.3900 |
| C17—C18 | 1.413 (12) | C31A—H31A | 0.9500 |
| C17—H17 | 0.9500 | C32A—C33A | 1.3900 |
| C18—C19 | 1.380 (13) | C32A—H32A | 0.9500 |
| C18—H18 | 0.9500 | C33A—C34A | 1.3900 |
| C19—C20 | 1.370 (14) | C33A—H33A | 0.9500 |

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|---|---|---|---|
| C19—H19 | 0.9500 | C34A—C35A | 1.3900 |
| C20—C21 | 1.378 (12) | C34A—H34A | 0.9500 |
| C20—H20 | 0.9500 | C35A—H35A | 0.9500 |
| C21—H21 | 0.9500 | | |

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| O3—Nd1—O4$^{i}$ | 136.30 (19) | C7—C6—C5 | 119.5 (11) |
| O3—Nd1—O5 | 70.64 (19) | C7—C6—H6 | 120.2 |
| O4$^{i}$—Nd1—O5 | 77.57 (18) | C5—C6—H6 | 120.2 |
| O3—Nd1—O2 | 72.27 (19) | C6—C7—C2 | 120.9 (10) |
| O4$^{i}$—Nd1—O2 | 145.82 (18) | C6—C7—H7 | 119.5 |
| O5—Nd1—O2 | 103.26 (18) | C2—C7—H7 | 119.5 |
| O3—Nd1—O11 | 125.9 (2) | O4—C8—O3 | 125.8 (8) |
| O4$^{i}$—Nd1—O11 | 73.60 (18) | O4—C8—C9A | 118.0 (8) |
| O5—Nd1—O11 | 78.40 (17) | O3—C8—C9A | 115.4 (9) |
| O2—Nd1—O11 | 73.18 (18) | O4—C8—C9 | 117.3 (8) |
| O3—Nd1—O6$^{i}$ | 86.92 (19) | O3—C8—C9 | 116.4 (9) |
| O4$^{i}$—Nd1—O6$^{i}$ | 86.44 (18) | C9A—C8—C9 | 17.2 (7) |
| O5—Nd1—O6$^{i}$ | 123.61 (17) | O6—C15—O5 | 119.0 (7) |
| O2—Nd1—O6$^{i}$ | 118.35 (17) | O6—C15—C16 | 122.6 (7) |
| O11—Nd1—O6$^{i}$ | 146.72 (17) | O5—C15—C16 | 118.4 (7) |
| O3—Nd1—O5$^{i}$ | 71.19 (19) | O6—C15—Nd1$^{i}$ | 59.7 (4) |
| O4$^{i}$—Nd1—O5$^{i}$ | 71.51 (17) | O5—C15—Nd1$^{i}$ | 60.4 (4) |
| O5—Nd1—O5$^{i}$ | 73.42 (19) | C16—C15—Nd1$^{i}$ | 170.4 (5) |
| O2—Nd1—O5$^{i}$ | 142.16 (17) | C17—C16—C21 | 120.7 (8) |
| O11—Nd1—O5$^{i}$ | 138.86 (17) | C17—C16—C15 | 118.4 (8) |
| O6$^{i}$—Nd1—O5$^{i}$ | 50.26 (16) | C21—C16—C15 | 121.0 (7) |
| O3—Nd1—O1 | 69.33 (18) | C16—C17—C18 | 120.1 (8) |
| O4$^{i}$—Nd1—O1 | 144.00 (17) | C16—C17—H17 | 120.0 |
| O5—Nd1—O1 | 137.46 (17) | C18—C17—H17 | 120.0 |
| O2—Nd1—O1 | 50.61 (17) | C19—C18—C17 | 118.3 (9) |
| O11—Nd1—O1 | 114.92 (18) | C19—C18—H18 | 120.8 |
| O6$^{i}$—Nd1—O1 | 67.75 (17) | C17—C18—H18 | 120.8 |
| O5$^{i}$—Nd1—O1 | 106.11 (17) | C20—C19—C18 | 120.9 (10) |
| O3—Nd1—Cl1 | 138.05 (15) | C20—C19—H19 | 119.5 |
| O4$^{i}$—Nd1—Cl1 | 79.01 (13) | C18—C19—H19 | 119.5 |
| O5—Nd1—Cl1 | 151.08 (13) | C19—C20—C21 | 120.9 (10) |
| O2—Nd1—Cl1 | 86.96 (13) | C19—C20—H20 | 119.5 |
| O11—Nd1—Cl1 | 78.90 (13) | C21—C20—H20 | 119.5 |
| O6$^{i}$—Nd1—Cl1 | 71.20 (12) | C20—C21—C16 | 119.0 (8) |
| O5$^{i}$—Nd1—Cl1 | 114.46 (12) | C20—C21—H21 | 120.5 |
| O1—Nd1—Cl1 | 69.34 (12) | C16—C21—H21 | 120.5 |
| O3—Nd1—C1 | 64.6 (2) | O7—C22—O8 | 119.3 (10) |
| O4$^{i}$—Nd1—C1 | 158.9 (2) | O7—C22—C23 | 121.7 (10) |
| O5—Nd1—C1 | 119.2 (2) | O8—C22—C23 | 118.9 (10) |
| O2—Nd1—C1 | 25.4 (2) | O7—C22—Nd2 | 54.6 (5) |
| O11—Nd1—C1 | 96.2 (2) | O8—C22—Nd2 | 67.1 (5) |
| O6$^{i}$—Nd1—C1 | 93.2 (2) | C23—C22—Nd2 | 165.5 (6) |
| O5$^{i}$—Nd1—C1 | 123.6 (2) | C24—C23—C28 | 121.4 (10) |
| O1—Nd1—C1 | 25.83 (19) | C24—C23—C22 | 121.4 (10) |

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| Cl1—Nd1—C1 | 80.90 (16) | C28—C23—C22 | 117.0 (11) |
| O3—Nd1—C15$^{i}$ | 80.8 (2) | C23—C24—C25 | 118.9 (11) |
| O4$^{i}$—Nd1—C15$^{i}$ | 75.3 (2) | C23—C24—H24 | 120.5 |
| O5—Nd1—C15$^{i}$ | 99.0 (2) | C25—C24—H24 | 120.5 |
| O2—Nd1—C15$^{i}$ | 136.5 (2) | C24—C25—C26 | 118.6 (13) |
| O11—Nd1—C15$^{i}$ | 148.63 (19) | C24—C25—H25 | 120.7 |
| O6$^{i}$—Nd1—C15$^{i}$ | 24.98 (18) | C26—C25—H25 | 120.7 |
| O5$^{i}$—Nd1—C15$^{i}$ | 25.58 (19) | C27—C26—C25 | 121.2 (13) |
| O1—Nd1—C15$^{i}$ | 88.4 (2) | C27—C26—H26 | 119.4 |
| Cl1—Nd1—C15$^{i}$ | 91.23 (16) | C25—C26—H26 | 119.4 |
| C1—Nd1—C15$^{i}$ | 111.7 (2) | C28—C27—C26 | 120.4 (14) |
| O3—Nd1—Nd2 | 94.43 (15) | C28—C27—H27 | 119.8 |
| O4$^{i}$—Nd1—Nd2 | 107.76 (13) | C26—C27—H27 | 119.8 |
| O5—Nd1—Nd2 | 160.61 (12) | C27—C28—C23 | 119.3 (13) |
| O2—Nd1—Nd2 | 82.92 (12) | C27—C28—H28 | 120.4 |
| O11—Nd1—Nd2 | 120.94 (13) | C23—C28—H28 | 120.4 |
| O6$^{i}$—Nd1—Nd2 | 40.66 (12) | O9—C29—O10 | 125.1 (7) |
| O5$^{i}$—Nd1—Nd2 | 90.33 (12) | O9—C29—C30 | 121.7 (10) |
| O1—Nd1—Nd2 | 36.76 (12) | O10—C29—C30 | 113.1 (9) |
| Cl1—Nd1—Nd2 | 46.03 (4) | O9—C29—C30A | 118.6 (9) |
| C1—Nd1—Nd2 | 61.10 (17) | O10—C29—C30A | 116.1 (9) |
| C15$^{i}$—Nd1—Nd2 | 65.57 (16) | C30—C29—C30A | 9.7 (12) |
| O8$^{ii}$—Nd2—O10$^{ii}$ | 79.77 (19) | O11—C36—C37 | 109.7 (8) |
| O8$^{ii}$—Nd2—O1 | 144.98 (19) | O11—C36—H36A | 109.7 |
| O10$^{ii}$—Nd2—O1 | 82.75 (18) | C37—C36—H36A | 109.7 |
| O8$^{ii}$—Nd2—O7 | 127.4 (2) | O11—C36—H36B | 109.7 |
| O10$^{ii}$—Nd2—O7 | 84.2 (2) | C37—C36—H36B | 109.7 |
| O1—Nd2—O7 | 80.1 (2) | H36A—C36—H36B | 108.2 |
| O8$^{ii}$—Nd2—O9 | 74.66 (19) | O12—C37—C36 | 110.5 (9) |
| O10$^{ii}$—Nd2—O9 | 136.64 (18) | O12—C37—H37A | 109.6 |
| O1—Nd2—O9 | 135.61 (19) | C36—C37—H37A | 109.6 |
| O7—Nd2—O9 | 84.3 (2) | O12—C37—H37B | 109.6 |
| O8$^{ii}$—Nd2—O6$^{i}$ | 74.84 (18) | C36—C37—H37B | 109.6 |
| O10$^{ii}$—Nd2—O6$^{i}$ | 73.25 (17) | H37A—C37—H37B | 108.1 |
| O1—Nd2—O6$^{i}$ | 71.14 (17) | O11—C38—C39 | 111.2 (9) |
| O7—Nd2—O6$^{i}$ | 145.2 (2) | O11—C38—H38A | 109.4 |
| O9—Nd2—O6$^{i}$ | 130.15 (18) | C39—C38—H38A | 109.4 |
| O8$^{ii}$—Nd2—O8 | 77.1 (2) | O11—C38—H38B | 109.4 |
| O10$^{ii}$—Nd2—O8 | 66.96 (17) | C39—C38—H38B | 109.4 |
| O1—Nd2—O8 | 122.75 (18) | H38A—C38—H38B | 108.0 |
| O7—Nd2—O8 | 50.7 (2) | O12—C39—C38 | 111.0 (10) |
| O9—Nd2—O8 | 73.49 (17) | O12—C39—H39A | 109.4 |
| O6$^{i}$—Nd2—O8 | 134.43 (17) | C38—C39—H39A | 109.4 |
| O8$^{ii}$—Nd2—Cl1 | 103.71 (14) | O12—C39—H39B | 109.4 |
| O10$^{ii}$—Nd2—Cl1 | 141.60 (14) | C38—C39—H39B | 109.4 |
| O1—Nd2—Cl1 | 72.87 (13) | H39A—C39—H39B | 108.0 |
| O7—Nd2—Cl1 | 119.06 (19) | C10—C9—C14 | 120.0 |
| O9—Nd2—Cl1 | 79.17 (13) | C10—C9—C8 | 120.3 (9) |
| O6$^{i}$—Nd2—Cl1 | 71.02 (12) | C14—C9—C8 | 119.3 (9) |

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| O8—Nd2—Cl1 | 151.44 (12) | C11—C10—C9 | 120.0 |
| O8$^{ii}$—Nd2—C22 | 103.1 (3) | C11—C10—H10 | 120.0 |
| O10$^{ii}$—Nd2—C22 | 70.4 (2) | C9—C10—H10 | 120.0 |
| O1—Nd2—C22 | 99.2 (2) | C10—C11—C12 | 120.0 |
| O7—Nd2—C22 | 25.3 (2) | C10—C11—H11 | 120.0 |
| O9—Nd2—C22 | 82.0 (2) | C12—C11—H11 | 120.0 |
| O6$^{i}$—Nd2—C22 | 143.3 (2) | C13—C12—C11 | 120.0 |
| O8—Nd2—C22 | 26.1 (2) | C13—C12—H12 | 120.0 |
| Cl1—Nd2—C22 | 141.6 (2) | C11—C12—H12 | 120.0 |
| O8$^{ii}$—Nd2—Nd1 | 111.13 (14) | C14—C13—C12 | 120.0 |
| O10$^{ii}$—Nd2—Nd1 | 96.31 (13) | C14—C13—H13 | 120.0 |
| O1—Nd2—Nd1 | 41.32 (13) | C12—C13—H13 | 120.0 |
| O7—Nd2—Nd1 | 120.26 (16) | C13—C14—C9 | 120.0 |
| O9—Nd2—Nd1 | 125.35 (13) | C13—C14—H14 | 120.0 |
| O6$^{i}$—Nd2—Nd1 | 40.19 (12) | C9—C14—H14 | 120.0 |
| O8—Nd2—Nd1 | 160.40 (12) | C10A—C9A—C14A | 120.0 |
| Cl1—Nd2—Nd1 | 46.23 (4) | C10A—C9A—C8 | 120.4 (8) |
| C22—Nd2—Nd1 | 140.4 (2) | C14A—C9A—C8 | 119.4 (8) |
| O8$^{ii}$—Nd2—Nd2$^{ii}$ | 41.74 (14) | C11A—C10A—C9A | 120.0 |
| O10$^{ii}$—Nd2—Nd2$^{ii}$ | 68.11 (13) | C11A—C10A—H10A | 120.0 |
| O1—Nd2—Nd2$^{ii}$ | 148.79 (13) | C9A—C10A—H10A | 120.0 |
| O7—Nd2—Nd2$^{ii}$ | 85.83 (16) | C10A—C11A—C12A | 120.0 |
| O9—Nd2—Nd2$^{ii}$ | 69.45 (13) | C10A—C11A—H11A | 120.0 |
| O6$^{i}$—Nd2—Nd2$^{ii}$ | 108.84 (12) | C12A—C11A—H11A | 120.0 |
| O8—Nd2—Nd2$^{ii}$ | 35.32 (13) | C13A—C12A—C11A | 120.0 |
| Cl1—Nd2—Nd2$^{ii}$ | 137.78 (5) | C13A—C12A—H12A | 120.0 |
| C22—Nd2—Nd2$^{ii}$ | 61.4 (2) | C11A—C12A—H12A | 120.0 |
| Nd1—Nd2—Nd2$^{ii}$ | 149.02 (2) | C12A—C13A—C14A | 120.0 |
| Nd2—Cl1—Nd1 | 87.74 (5) | C12A—C13A—H13A | 120.0 |
| C1—O1—Nd2 | 153.5 (5) | C14A—C13A—H13A | 120.0 |
| C1—O1—Nd1 | 89.1 (5) | C13A—C14A—C9A | 120.0 |
| Nd2—O1—Nd1 | 101.92 (19) | C13A—C14A—H14A | 120.0 |
| C1—O2—Nd1 | 97.6 (5) | C9A—C14A—H14A | 120.0 |
| C8—O3—Nd1 | 143.1 (6) | C31—C30—C35 | 120.0 |
| C8—O4—Nd1$^{i}$ | 134.2 (5) | C31—C30—C29 | 118.9 (11) |
| C15—O5—Nd1 | 159.1 (5) | C35—C30—C29 | 121.0 (11) |
| C15—O5—Nd1$^{i}$ | 94.0 (5) | C32—C31—C30 | 120.0 |
| Nd1—O5—Nd1$^{i}$ | 106.58 (19) | C32—C31—H31 | 120.0 |
| C15—O6—Nd1$^{i}$ | 95.3 (5) | C30—C31—H31 | 120.0 |
| C15—O6—Nd2$^{i}$ | 164.7 (5) | C31—C32—C33 | 120.0 |
| Nd1$^{i}$—O6—Nd2$^{i}$ | 99.15 (18) | C31—C32—H32 | 120.0 |
| C22—O7—Nd2 | 100.2 (6) | C33—C32—H32 | 120.0 |
| C22—O8—Nd2$^{ii}$ | 169.6 (7) | C32—C33—C34 | 120.0 |
| C22—O8—Nd2 | 86.8 (6) | C32—C33—H33 | 120.0 |
| Nd2$^{ii}$—O8—Nd2 | 102.9 (2) | C34—C33—H33 | 120.0 |
| C29—O9—Nd2 | 135.2 (5) | C33—C34—C35 | 120.0 |
| C29—O10—Nd2$^{ii}$ | 139.3 (5) | C33—C34—H34 | 120.0 |
| C36—O11—C38 | 109.3 (7) | C35—C34—H34 | 120.0 |
| C36—O11—Nd1 | 128.6 (5) | C34—C35—C30 | 120.0 |

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| C38—O11—Nd1 | 122.1 (5) | C34—C35—H35 | 120.0 |
| C39—O12—C37 | 105.8 (8) | C30—C35—H35 | 120.0 |
| O2—C1—O1 | 119.9 (8) | C31A—C30A—C35A | 120.0 |
| O2—C1—C2 | 120.4 (8) | C31A—C30A—C29 | 122.2 (10) |
| O1—C1—C2 | 119.5 (8) | C35A—C30A—C29 | 117.7 (10) |
| O2—C1—Nd1 | 57.0 (4) | C32A—C31A—C30A | 120.0 |
| O1—C1—Nd1 | 65.1 (4) | C32A—C31A—H31A | 120.0 |
| C2—C1—Nd1 | 160.5 (5) | C30A—C31A—H31A | 120.0 |
| C7—C2—C3 | 119.5 (8) | C31A—C32A—C33A | 120.0 |
| C7—C2—C1 | 118.6 (8) | C31A—C32A—H32A | 120.0 |
| C3—C2—C1 | 121.8 (8) | C33A—C32A—H32A | 120.0 |
| C4—C3—C2 | 119.6 (9) | C34A—C33A—C32A | 120.0 |
| C4—C3—H3 | 120.2 | C34A—C33A—H33A | 120.0 |
| C2—C3—H3 | 120.2 | C32A—C33A—H33A | 120.0 |
| C5—C4—C3 | 120.4 (9) | C33A—C34A—C35A | 120.0 |
| C5—C4—H4 | 119.8 | C33A—C34A—H34A | 120.0 |
| C3—C4—H4 | 119.8 | C35A—C34A—H34A | 120.0 |
| C4—C5—C6 | 120.0 (10) | C34A—C35A—C30A | 120.0 |
| C4—C5—H5 | 120.0 | C34A—C35A—H35A | 120.0 |
| C6—C5—H5 | 120.0 | C30A—C35A—H35A | 120.0 |

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1.