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catena-Poly[[aqua[(2,4-dichlorophenoxy)acetato]neodymium(III)]-di-μ-(2,4-dichlorophenoxy)acetato]

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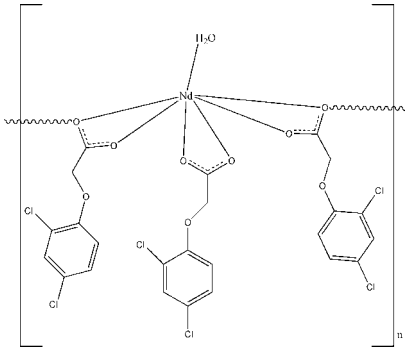
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.031; wR factor = 0.087; data-to-parameter ratio = 15.2.

The title complex, $[Nd(C_8H_5Cl_2O_3)_3(H_2O)]_n$, is a neodymium polymer based on the flexible 2,4-dichlorophenoxyacetate ligand. The Nd^{II} center is coordinated by eight O atoms from five 2,4-dichlorophenoxyacetate ligands and one water molecule, and displays a distorted tricapped trigonal–prismatic geometry. The Nd centers are linked by the (2,4-dichlorophenoxy)acetate ligands *via* two bridging carboxylate O atoms, with an Nd···Nd distance of 4.172 (3) Å, forming chains along the *c* axis. The chains are assembled into ruffled layers *via* π–π stacking interactions; the centroid–centroid and offset distances between phenyl groups [at $(-1+x, y, -1+z)$] are 3.719 (2) and 0.060 (2) Å, respectively, indicating a normal π–π stacking interaction.

Related literature

Related literature: Dendrinou-Samara *et al.* (2001); Lee *et al.* (2007); Psomas *et al.* (2000).



Experimental

Crystal data

$[Nd(C_8H_5Cl_2O_3)_3(H_2O)]$
M_r = 822.32
Monoclinic, $P2_1/c$
a = 10.1801 (2) Å
b = 35.4768 (6) Å
c = 8.1456 (2) Å
β = 97.144 (1)°
V = 2919.00 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.38 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.566, T_{max} = 0.626
31522 measured reflections
5617 independent reflections
5062 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.088
S = 1.23
5617 reflections
370 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −1.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O8^{i}	0.811 (19)	1.98 (3)	2.702 (4)	148 (4)
O1W—H2W···Cl5^{i}	0.807 (19)	2.89 (4)	3.422 (4)	125 (4)
O1W—H2W···O7^{ii}	0.807 (19)	2.66 (2)	3.395 (5)	152 (4)

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2021).

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supplementary materials

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catena-Poly[[aqua[(2,4-dichlorophenoxy)acetato]neodymium(III)]-di-μ-(2,4-dichlorophenoxy)acetato]

J. Guo, W.-J. Liang and W.-D. Song

Comment

2,4-Dichlorophenoxyacetic acid is an important biologically active compound that has been commonly used in herbicides and plant-growth agents. The monophenoxyacetate group has versatile bonding modes to metal ions and easily forms simple complexes (Dendrinou-Samara *et al.*, 2001; Psomas *et al.*, 2000). Recently, we obtained the one-dimensional neodymium polymer (I), its crystal structure is reported here.

The Nd^{III} centre is in a distorted tricapped trigonal prismatic geometry, defined by eight O atoms from five 2,4-dichlorophenoxyacetate ligands and one water molecule (Fig. 1). Coordination bond lengths, angles and torsion angles at the Nd^{III} atom are given in Table 1. The 2,4-dichlorophenoxyacetate ligands exhibit two different types of coordination modes: One of the ligands is coordinating only to one of the neodymium centers (O7, O8), the other two carboxylate ligands are linking the neodym centers in a μ_2 way *via* the carboxylate atoms

O2 and O4 to form chains parallel to the *c* axis with a Nd···Nd distance of 4.172 (3) Å. The oxygen atoms of the non-bridging 2,4-dichlorophenoxyacetate ligand are forming hydrogen bonds with the coordinated water molecules of neighboring entities with the H-bonds extending parallel to the main polymeric chain (see Table 2 for numerical values). The chains as a whole are also involved in π···π stacking interactions of some of the phenyl rings (C11 to C16) with neigboring chains to form a ruffly layer perpendicular to the *b* axis (Fig. 2). The centroid-centroid distance between phenyl groups (at $-1+x, y, -1+z$) and the offset are 3.719 (2) and 0.060 (2) Å, respectively, indicating a normal π···π stacking interaction (Lee *et al.*, 2007).

Experimental

A mixture of Nd_2O_3 (0.5 mmol), 2,4-dichlorophenoxyacetic acid (1 mmol) and H_2O (10 ml) in the presence of $HClO_4$ (0.385 mmol) was stirred vigorously for 20 min and then sealed in a Teflon-lined stainless-steel autoclave (20 ml, capacity). The autoclave was heated to and maintained at 433 K for 7 days, and then cooled to room temperature at 5 K h^{-1}. The crystal were obtained in *ca* 46% yield based on Nd.

Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å, and with U_{iso}(H) = 1.2 U_{eq}(C). Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.85 Å and H···H = 1.39 Å, each within a standard deviation of 0.01 Å

Figures

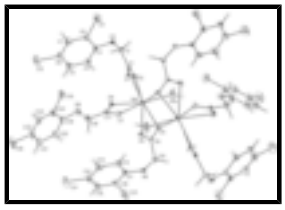

Fig. 1. The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Unlabeled atoms are related to the labelled atoms by the symmetry operator (x, $0.5 - y$, $-1/2 + z$).

Fig. 2. A packing view of (I) along the *c* axis. Hydrogen bonds are depicted as broken lines.

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Crystal data

$[Nd(C_8H_5Cl_2O_3)_3(H_2O)]$	F_{000} = 1612
M_r = 822.32	D_x = 1.871 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8000 reflections
a = 10.1801 (2) Å	θ = 1.7–26.0º
b = 35.4768 (6) Å	μ = 2.38 mm^{-1}
c = 8.1456 (2) Å	T = 293 (2) K
β = 97.144 (1)º	Platelet, purple
V = 2919.00 (10) Å^3	0.25 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	5617 independent reflections
Radiation source: fine-focus sealed tube	5062 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 293(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12
T_{min} = 0.566, T_{max} = 0.626	k = −43→43
31522 measured reflections	l = −10→8

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.031	H atoms treated by a mixture of

	independent and constrained refinement
$wR(F^2) = 0.088$	$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 2.8846P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.23$	$(\Delta/\sigma)_{max} = 0.001$
5617 reflections	$\Delta\rho_{max} = 0.74$ e Å^{-3}
370 parameters	$\Delta\rho_{min} = -1.54$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2331 (3)	0.23189 (10)	0.4591 (5)	0.0211 (8)
C2	0.1116 (4)	0.22703 (12)	0.3335 (5)	0.0310 (9)
H2A	0.0752	0.2516	0.3022	0.037*
H2B	0.1370	0.2151	0.2350	0.037*
C3	0.0273 (4)	0.16667 (11)	0.3963 (5)	0.0284 (8)
C4	0.1374 (4)	0.14754 (13)	0.3584 (6)	0.0456 (12)
H4	0.2118	0.1609	0.3359	0.055*
C5	0.1378 (5)	0.10843 (14)	0.3535 (8)	0.0592 (15)
H5	0.2119	0.0957	0.3260	0.071*
C6	0.0302 (5)	0.08870 (13)	0.3888 (8)	0.0546 (13)
C7	−0.0803 (4)	0.10688 (13)	0.4312 (7)	0.0470 (12)
H7	−0.1530	0.0932	0.4570	0.056*
C8	−0.0809 (4)	0.14578 (12)	0.4346 (5)	0.0337 (9)
C9	0.7044 (3)	0.22777 (10)	0.9310 (5)	0.0234 (8)
C10	0.8244 (4)	0.22184 (12)	1.0600 (5)	0.0300 (9)
H10A	0.8602	0.2462	1.0970	0.036*
H10B	0.7969	0.2089	1.1550	0.036*
C11	0.9044 (4)	0.16244 (11)	0.9735 (5)	0.0298 (9)
C12	0.7919 (4)	0.14320 (13)	1.0026 (6)	0.0422 (11)
H12	0.7219	0.1563	1.0389	0.051*
C13	0.7817 (5)	0.10486 (15)	0.9785 (7)	0.0569 (14)
H13	0.7057	0.0923	1.0003	0.068*
C14	0.8829 (6)	0.08520 (14)	0.9227 (8)	0.0597 (15)

C15	0.9975 (5)	0.10342 (14)	0.8931 (7)	0.0536 (13)
H15	1.0669	0.0900	0.8569	0.064*
C16	1.0074 (4)	0.14191 (13)	0.9182 (6)	0.0400 (10)
C17	0.4793 (3)	0.15799 (11)	0.6587 (5)	0.0292 (9)
C18	0.5042 (5)	0.11663 (12)	0.6386 (6)	0.0456 (11)
H18A	0.5941	0.1105	0.6851	0.055*
H18B	0.4440	0.1021	0.6972	0.055*
C19	0.5380 (4)	0.07433 (12)	0.4211 (6)	0.0426 (11)
C20	0.6068 (5)	0.04845 (12)	0.5265 (7)	0.0518 (13)
H20	0.6182	0.0528	0.6399	0.062*
C21	0.6589 (5)	0.01595 (14)	0.4636 (9)	0.0635 (16)
H21	0.7055	−0.0012	0.5348	0.076*
C22	0.6413 (6)	0.00947 (13)	0.2979 (9)	0.0632 (16)
C23	0.5724 (6)	0.03446 (14)	0.1902 (8)	0.0604 (15)
H23	0.5605	0.0297	0.0770	0.072*
C24	0.5212 (5)	0.06667 (13)	0.2532 (7)	0.0493 (12)
Cl1	−0.21982 (12)	0.16884 (4)	0.4836 (2)	0.0636 (4)
Cl2	0.02712 (19)	0.03967 (4)	0.3748 (3)	0.1027 (7)
Cl3	1.15126 (13)	0.16473 (4)	0.8836 (2)	0.0710 (4)
Cl4	0.8703 (2)	0.03676 (4)	0.8933 (3)	0.1017 (7)
Cl5	0.43592 (16)	0.09847 (4)	0.11576 (19)	0.0678 (4)
Cl6	0.7043 (2)	−0.03135 (4)	0.2194 (3)	0.1014 (7)
Nd1	0.469125 (17)	0.237244 (5)	0.69698 (2)	0.01875 (8)
O1	0.2348 (2)	0.21996 (8)	0.6017 (3)	0.0319 (6)
O2	0.3345 (2)	0.24889 (8)	0.4157 (3)	0.0265 (6)
O3	0.0130 (2)	0.20488 (7)	0.3960 (4)	0.0309 (6)
O4	0.6009 (3)	0.24198 (8)	0.9835 (3)	0.0290 (4)
O5	0.7074 (2)	0.22086 (8)	0.7852 (3)	0.0290 (4)
O6	0.9254 (2)	0.20022 (8)	0.9956 (3)	0.0318 (6)
O7	0.4680 (3)	0.17038 (8)	0.8010 (4)	0.0334 (6)
O8	0.4773 (3)	0.17940 (7)	0.5340 (3)	0.0320 (6)
O9	0.4849 (3)	0.10728 (8)	0.4683 (4)	0.0457 (8)
O1W	0.4630 (4)	0.30741 (9)	0.7056 (4)	0.0515 (9)
H1W	0.469 (6)	0.3196 (12)	0.790 (3)	0.062*
H2W	0.459 (6)	0.3203 (12)	0.623 (3)	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0169 (16)	0.0262 (18)	0.019 (2)	−0.0013 (13)	−0.0007 (13)	−0.0043 (15)
C2	0.0232 (18)	0.038 (2)	0.030 (2)	−0.0101 (15)	−0.0027 (16)	0.0029 (18)
C3	0.0244 (17)	0.036 (2)	0.023 (2)	−0.0037 (15)	−0.0033 (15)	−0.0031 (17)
C4	0.028 (2)	0.047 (3)	0.063 (3)	−0.0041 (18)	0.007 (2)	−0.008 (2)
C5	0.039 (3)	0.050 (3)	0.089 (5)	0.009 (2)	0.015 (3)	−0.014 (3)
C6	0.052 (3)	0.035 (3)	0.076 (4)	0.002 (2)	0.005 (3)	−0.002 (3)
C7	0.038 (2)	0.043 (3)	0.061 (3)	−0.0049 (19)	0.012 (2)	0.007 (2)
C8	0.031 (2)	0.039 (2)	0.032 (3)	−0.0024 (16)	0.0099 (17)	0.0012 (19)
C9	0.0224 (17)	0.0220 (17)	0.026 (2)	−0.0018 (13)	0.0043 (15)	0.0018 (15)

C10	0.0260 (18)	0.038 (2)	0.024 (2)	0.0082 (16)	−0.0042 (15)	−0.0044 (17)
C11	0.0283 (18)	0.038 (2)	0.023 (2)	0.0069 (16)	0.0002 (15)	0.0042 (17)
C12	0.033 (2)	0.048 (3)	0.046 (3)	0.0035 (18)	0.0047 (19)	0.005 (2)
C13	0.047 (3)	0.054 (3)	0.069 (4)	−0.005 (2)	0.005 (2)	0.010 (3)
C14	0.076 (4)	0.035 (3)	0.065 (4)	0.003 (2)	−0.005 (3)	0.002 (2)
C15	0.059 (3)	0.045 (3)	0.059 (4)	0.019 (2)	0.013 (3)	−0.002 (2)
C16	0.037 (2)	0.046 (3)	0.038 (3)	0.0091 (19)	0.0081 (19)	0.007 (2)
C17	0.0269 (18)	0.0267 (19)	0.034 (3)	0.0001 (14)	0.0028 (16)	0.0013 (18)
C18	0.064 (3)	0.029 (2)	0.044 (3)	0.001 (2)	0.006 (2)	0.002 (2)
C19	0.043 (2)	0.030 (2)	0.057 (3)	−0.0062 (18)	0.013 (2)	−0.010 (2)
C20	0.058 (3)	0.030 (2)	0.066 (4)	0.001 (2)	0.005 (2)	−0.002 (2)
C21	0.059 (3)	0.036 (3)	0.096 (5)	0.004 (2)	0.010 (3)	−0.002 (3)
C22	0.065 (3)	0.030 (3)	0.101 (5)	−0.002 (2)	0.032 (3)	−0.016 (3)
C23	0.076 (4)	0.041 (3)	0.068 (4)	−0.004 (3)	0.025 (3)	−0.014 (3)
C24	0.054 (3)	0.034 (2)	0.062 (4)	−0.005 (2)	0.016 (2)	−0.004 (2)
Cl1	0.0447 (6)	0.0503 (7)	0.1041 (12)	0.0008 (5)	0.0424 (7)	0.0047 (7)
Cl2	0.0892 (12)	0.0357 (8)	0.184 (2)	0.0034 (7)	0.0217 (12)	−0.0074 (10)
Cl3	0.0502 (7)	0.0626 (8)	0.1090 (13)	0.0091 (6)	0.0447 (8)	0.0078 (8)
Cl4	0.1212 (15)	0.0392 (8)	0.1399 (19)	0.0014 (9)	−0.0025 (13)	−0.0050 (9)
Cl5	0.0964 (11)	0.0528 (8)	0.0534 (9)	0.0074 (7)	0.0063 (7)	−0.0100 (7)
Cl6	0.1208 (15)	0.0460 (8)	0.1457 (19)	0.0169 (9)	0.0498 (13)	−0.0285 (10)
Nd1	0.02001 (11)	0.02489 (12)	0.01098 (13)	−0.00004 (7)	0.00042 (7)	0.00037 (7)
O1	0.0294 (13)	0.0506 (17)	0.0148 (15)	−0.0125 (12)	−0.0001 (10)	0.0018 (13)
O2	0.0164 (11)	0.0347 (13)	0.0280 (16)	−0.0028 (10)	0.0016 (10)	−0.0024 (12)
O3	0.0204 (12)	0.0331 (15)	0.0389 (18)	−0.0065 (10)	0.0019 (11)	0.0011 (13)
O4	0.0265 (9)	0.0502 (12)	0.0100 (10)	0.0078 (8)	0.0011 (7)	−0.0052 (9)
O5	0.0265 (9)	0.0502 (12)	0.0100 (10)	0.0078 (8)	0.0011 (7)	−0.0052 (9)
O6	0.0221 (12)	0.0384 (15)	0.0341 (17)	0.0068 (11)	0.0009 (11)	−0.0033 (13)
O7	0.0439 (16)	0.0305 (14)	0.0259 (17)	−0.0006 (12)	0.0047 (12)	0.0042 (12)
O8	0.0422 (15)	0.0278 (14)	0.0263 (16)	0.0043 (11)	0.0051 (12)	−0.0006 (12)
O9	0.0546 (19)	0.0334 (16)	0.048 (2)	0.0087 (14)	0.0006 (15)	−0.0100 (15)
O1W	0.091 (3)	0.0291 (17)	0.035 (2)	0.0007 (16)	0.012 (2)	−0.0003 (14)

Geometric parameters (Å, °)

C1—O1	1.235 (5)	C15—H15	0.9300
C1—O2	1.282 (4)	C16—Cl3	1.727 (5)
C1—C2	1.514 (5)	C17—O7	1.258 (5)
C2—O3	1.418 (4)	C17—O8	1.266 (5)
C2—H2A	0.9700	C17—C18	1.501 (6)
C2—H2B	0.9700	C18—O9	1.416 (6)
C3—O3	1.364 (5)	C18—H18A	0.9700
C3—C4	1.378 (6)	C18—H18B	0.9700
C3—C8	1.394 (5)	C19—O9	1.363 (5)
C4—C5	1.388 (7)	C19—C24	1.384 (7)
C4—H4	0.9300	C19—C20	1.386 (7)
C5—C6	1.361 (7)	C20—C21	1.393 (7)
C5—H5	0.9300	C20—H20	0.9300
C6—C7	1.377 (7)	C21—C22	1.359 (9)

C6—Cl2	1.743 (5)	C21—H21	0.9300
C7—C8	1.380 (6)	C22—C23	1.376 (8)
C7—H7	0.9300	C22—Cl6	1.738 (5)
C8—Cl1	1.724 (4)	C23—C24	1.381 (7)
C9—O5	1.217 (5)	C23—H23	0.9300
C9—O4	1.288 (4)	C24—Cl5	1.743 (6)
C9—C10	1.524 (5)	Nd1—O2^{i}	2.430 (3)
C10—O6	1.434 (4)	Nd1—O4^{ii}	2.439 (3)
C10—H10A	0.9700	Nd1—O8	2.451 (3)
C10—H10B	0.9700	Nd1—O1W	2.491 (3)
C11—O6	1.366 (5)	Nd1—O1	2.492 (2)
C11—C12	1.379 (6)	Nd1—O5	2.511 (2)
C11—C16	1.396 (6)	Nd1—O7	2.519 (3)
C12—C13	1.376 (7)	Nd1—O4	2.549 (3)
C12—H12	0.9300	Nd1—O2	2.553 (3)
C13—C14	1.367 (8)	O2—Nd1^{ii}	2.430 (3)
C13—H13	0.9300	O4—Nd1^{i}	2.439 (3)
C14—C15	1.381 (8)	O1W—H1W	0.811 (19)
C14—Cl4	1.737 (5)	O1W—H2W	0.807 (19)
C15—C16	1.382 (7)		
O1—C1—O2	120.2 (3)	C19—C20—H20	119.8
O1—C1—C2	120.8 (3)	C21—C20—H20	119.8
O2—C1—C2	119.0 (3)	C22—C21—C20	119.7 (5)
O3—C2—C1	112.1 (3)	C22—C21—H21	120.1
O3—C2—H2A	109.2	C20—C21—H21	120.1
C1—C2—H2A	109.2	C21—C22—C23	121.2 (5)
O3—C2—H2B	109.2	C21—C22—Cl6	119.8 (5)
C1—C2—H2B	109.2	C23—C22—Cl6	119.0 (5)
H2A—C2—H2B	107.9	C22—C23—C24	118.8 (6)
O3—C3—C4	125.4 (4)	C22—C23—H23	120.6
O3—C3—C8	116.2 (3)	C24—C23—H23	120.6
C4—C3—C8	118.4 (4)	C23—C24—C19	121.6 (5)
C3—C4—C5	120.3 (4)	C23—C24—Cl5	118.5 (5)
C3—C4—H4	119.9	C19—C24—Cl5	119.9 (4)
C5—C4—H4	119.9	O2^{i}—Nd1—O4^{ii}	150.72 (10)
C6—C5—C4	120.2 (4)	O2^{i}—Nd1—O8	128.82 (9)
C6—C5—H5	119.9	O4^{ii}—Nd1—O8	78.94 (9)
C4—C5—H5	119.9	O2^{i}—Nd1—O1W	76.03 (11)
C5—C6—C7	121.1 (4)	O4^{ii}—Nd1—O1W	74.69 (11)
C5—C6—Cl2	120.5 (4)	O8—Nd1—O1W	148.70 (10)
C7—C6—Cl2	118.4 (4)	O2^{i}—Nd1—O1	70.88 (9)
C6—C7—C8	118.6 (4)	O4^{ii}—Nd1—O1	116.28 (9)
C6—C7—H7	120.7	O8—Nd1—O1	73.80 (9)
C8—C7—H7	120.7	O1W—Nd1—O1	103.20 (11)
C7—C8—C3	121.4 (4)	O2^{i}—Nd1—O5	116.76 (8)
C7—C8—Cl1	119.0 (3)	O4^{ii}—Nd1—O5	71.11 (9)

C3—C8—Cl1	119.6 (3)	O8—Nd1—O5	82.21 (9)
O5—C9—O4	121.6 (3)	O1W—Nd1—O5	104.47 (11)
O5—C9—C10	122.0 (3)	O1—Nd1—O5	152.33 (10)
O4—C9—C10	116.3 (3)	$O2^{i}$—Nd1—O7	85.27 (9)
O6—C10—C9	111.8 (3)	$O4^{ii}$—Nd1—O7	123.39 (9)
O6—C10—H10A	109.3	O8—Nd1—O7	52.82 (9)
C9—C10—H10A	109.3	O1W—Nd1—O7	158.46 (10)
O6—C10—H10B	109.3	O1—Nd1—O7	80.13 (9)
C9—C10—H10B	109.3	O5—Nd1—O7	74.37 (9)
H10A—C10—H10B	107.9	$O2^{i}$—Nd1—O4	66.17 (8)
O6—C11—C12	125.6 (4)	$O4^{ii}$—Nd1—O4	111.05 (9)
O6—C11—C16	116.3 (4)	O8—Nd1—O4	120.11 (9)
C12—C11—C16	118.1 (4)	O1W—Nd1—O4	85.44 (10)
C13—C12—C11	120.9 (4)	O1—Nd1—O4	132.52 (9)
C13—C12—H12	119.5	O5—Nd1—O4	51.21 (8)
C11—C12—H12	119.5	O7—Nd1—O4	77.18 (9)
C14—C13—C12	120.3 (5)	$O2^{i}$—Nd1—O2	109.66 (8)
C14—C13—H13	119.8	$O4^{ii}$—Nd1—O2	65.98 (8)
C12—C13—H13	119.8	O8—Nd1—O2	72.55 (9)
C13—C14—C15	120.4 (5)	O1W—Nd1—O2	81.43 (10)
C13—C14—Cl4	120.3 (5)	O1—Nd1—O2	51.24 (8)
C15—C14—Cl4	119.2 (4)	O5—Nd1—O2	133.31 (8)
C14—C15—C16	119.0 (5)	O7—Nd1—O2	115.44 (9)
C14—C15—H15	120.5	O4—Nd1—O2	166.86 (9)
C16—C15—H15	120.5	C1—O1—Nd1	96.3 (2)
C15—C16—C11	121.3 (4)	C1—O2—$Nd1^{ii}$	147.6 (2)
C15—C16—Cl3	119.1 (4)	C1—O2—Nd1	92.1 (2)
C11—C16—Cl3	119.6 (3)	$Nd1^{ii}$—O2—Nd1	113.70 (9)
O7—C17—O8	122.3 (4)	C3—O3—C2	118.1 (3)
O7—C17—C18	118.6 (4)	C9—O4—$Nd1^{i}$	154.2 (2)
O8—C17—C18	119.0 (4)	C9—O4—Nd1	91.6 (2)
O9—C18—C17	109.3 (4)	$Nd1^{i}$—O4—Nd1	113.52 (10)
O9—C18—H18A	109.8	C9—O5—Nd1	95.3 (2)
C17—C18—H18A	109.8	C11—O6—C10	117.8 (3)
O9—C18—H18B	109.8	C17—O7—Nd1	90.8 (2)
C17—C18—H18B	109.8	C17—O8—Nd1	93.8 (2)
H18A—C18—H18B	108.3	C19—O9—C18	117.7 (4)
O9—C19—C24	116.3 (4)	Nd1—O1W—H1W	124 (3)
O9—C19—C20	125.6 (5)	Nd1—O1W—H2W	123 (3)
C24—C19—C20	118.2 (4)	H1W—O1W—H2W	113 (3)
C19—C20—C21	120.5 (5)		
O1—C1—C2—O3	−5.7 (5)	$O2^{i}$—Nd1—O2—$Nd1^{ii}$	155.20 (14)
O2—C1—C2—O3	174.8 (3)	$O4^{ii}$—Nd1—O2—$Nd1^{ii}$	6.46 (9)
O3—C3—C4—C5	−176.3 (5)	O8—Nd1—O2—$Nd1^{ii}$	−78.96 (12)
C8—C3—C4—C5	2.1 (7)	O1W—Nd1—O2—$Nd1^{ii}$	83.44 (13)
C3—C4—C5—C6	−1.1 (9)	O1—Nd1—O2—$Nd1^{ii}$	−161.91 (17)

C4—C5—C6—C7	−0.5 (9)	O5—Nd1—O2—Nd1^{ii}	−18.41 (18)
C4—C5—C6—Cl2	177.4 (5)	O7—Nd1—O2—Nd1^{ii}	−110.62 (11)
C5—C6—C7—C8	1.1 (9)	O4—Nd1—O2—Nd1^{ii}	86.1 (3)
Cl2—C6—C7—C8	−176.9 (4)	C4—C3—O3—C2	7.8 (6)
C6—C7—C8—C3	0.0 (8)	C8—C3—O3—C2	−170.5 (3)
C6—C7—C8—Cl1	178.8 (4)	C1—C2—O3—C3	−79.9 (4)
O3—C3—C8—C7	176.9 (4)	O5—C9—O4—Nd1^{i}	173.1 (4)
C4—C3—C8—C7	−1.6 (7)	C10—C9—O4—Nd1^{i}	−9.7 (7)
O3—C3—C8—Cl1	−1.8 (5)	O5—C9—O4—Nd1	5.1 (4)
C4—C3—C8—Cl1	179.7 (3)	C10—C9—O4—Nd1	−177.7 (3)
O5—C9—C10—O6	−12.6 (5)	O2^{i}—Nd1—O4—C9	167.9 (2)
O4—C9—C10—O6	170.1 (3)	O4^{ii}—Nd1—O4—C9	−43.72 (17)
O6—C11—C12—C13	−179.0 (4)	O8—Nd1—O4—C9	45.5 (2)
C16—C11—C12—C13	0.3 (7)	O1W—Nd1—O4—C9	−115.4 (2)
C11—C12—C13—C14	−1.0 (8)	O1—Nd1—O4—C9	140.9 (2)
C12—C13—C14—C15	1.3 (9)	O5—Nd1—O4—C9	−2.70 (19)
C12—C13—C14—Cl4	179.7 (4)	O7—Nd1—O4—C9	77.4 (2)
C13—C14—C15—C16	−1.0 (8)	O2—Nd1—O4—C9	−118.1 (3)
Cl4—C14—C15—C16	−179.4 (4)	O2^{i}—Nd1—O4—Nd1^{i}	−6.45 (9)
C14—C15—C16—C11	0.4 (8)	O4^{ii}—Nd1—O4—Nd1^{i}	141.95 (15)
C14—C15—C16—Cl3	179.3 (4)	O8—Nd1—O4—Nd1^{i}	−128.87 (11)
O6—C11—C16—C15	179.3 (4)	O1W—Nd1—O4—Nd1^{i}	70.29 (13)
C12—C11—C16—C15	0.0 (7)	O1—Nd1—O4—Nd1^{i}	−33.46 (18)
O6—C11—C16—Cl3	0.5 (5)	O5—Nd1—O4—Nd1^{i}	−177.03 (17)
C12—C11—C16—Cl3	−178.9 (3)	O7—Nd1—O4—Nd1^{i}	−96.91 (12)
O7—C17—C18—O9	167.3 (3)	O2—Nd1—O4—Nd1^{i}	67.6 (4)
O8—C17—C18—O9	−16.3 (5)	O4—C9—O5—Nd1	−5.2 (4)
O9—C19—C20—C21	−178.8 (4)	C10—C9—O5—Nd1	177.7 (3)
C24—C19—C20—C21	0.9 (7)	O2^{i}—Nd1—O5—C9	−6.8 (2)
C19—C20—C21—C22	−0.5 (8)	O4^{ii}—Nd1—O5—C9	142.5 (2)
C20—C21—C22—C23	−0.1 (8)	O8—Nd1—O5—C9	−136.6 (2)
C20—C21—C22—Cl6	−179.2 (4)	O1W—Nd1—O5—C9	74.6 (2)
C21—C22—C23—C24	0.3 (8)	O1—Nd1—O5—C9	−106.7 (3)
Cl6—C22—C23—C24	179.3 (4)	O7—Nd1—O5—C9	−83.1 (2)
C22—C23—C24—C19	0.2 (8)	O4—Nd1—O5—C9	2.9 (2)
C22—C23—C24—Cl5	179.2 (4)	O2—Nd1—O5—C9	166.5 (2)
O9—C19—C24—C23	178.9 (4)	C12—C11—O6—C10	2.3 (6)
C20—C19—C24—C23	−0.8 (7)	C16—C11—O6—C10	−177.0 (4)
O9—C19—C24—Cl5	0.0 (6)	C9—C10—O6—C11	−73.9 (4)
C20—C19—C24—Cl5	−179.7 (4)	O8—C17—O7—Nd1	−4.8 (4)
O2—C1—O1—Nd1	−3.9 (4)	C18—C17—O7—Nd1	171.5 (3)
C2—C1—O1—Nd1	176.7 (3)	O2^{i}—Nd1—O7—C17	151.1 (2)
O2^{i}—Nd1—O1—C1	139.4 (2)	O4^{ii}—Nd1—O7—C17	−35.4 (2)
O4^{ii}—Nd1—O1—C1	−9.7 (3)	O8—Nd1—O7—C17	2.6 (2)
O8—Nd1—O1—C1	−78.2 (2)	O1W—Nd1—O7—C17	−179.3 (3)

O1W—Nd1—O1—C1	69.5 (2)	O1—Nd1—O7—C17	79.7 (2)
O5—Nd1—O1—C1	−109.2 (3)	O5—Nd1—O7—C17	−89.4 (2)
O7—Nd1—O1—C1	−132.2 (2)	O4—Nd1—O7—C17	−142.3 (2)
O4—Nd1—O1—C1	165.5 (2)	O2—Nd1—O7—C17	41.6 (2)
O2—Nd1—O1—C1	2.1 (2)	O7—C17—O8—Nd1	4.9 (4)
O1—C1—O2—Nd1^{ii}	147.7 (3)	C18—C17—O8—Nd1	−171.4 (3)
C2—C1—O2—Nd1^{ii}	−32.8 (6)	O2^{i}—Nd1—O8—C17	−44.6 (2)
O1—C1—O2—Nd1	3.7 (4)	O4^{ii}—Nd1—O8—C17	145.8 (2)
C2—C1—O2—Nd1	−176.8 (3)	O1W—Nd1—O8—C17	178.8 (2)
O2^{i}—Nd1—O2—C1	−44.94 (17)	O1—Nd1—O8—C17	−92.4 (2)
O4^{ii}—Nd1—O2—C1	166.3 (2)	O5—Nd1—O8—C17	73.7 (2)
O8—Nd1—O2—C1	80.9 (2)	O7—Nd1—O8—C17	−2.6 (2)
O1W—Nd1—O2—C1	−116.7 (2)	O4—Nd1—O8—C17	37.8 (2)
O1—Nd1—O2—C1	−2.06 (19)	O2—Nd1—O8—C17	−146.1 (2)
O5—Nd1—O2—C1	141.5 (2)	C24—C19—O9—C18	−177.9 (4)
O7—Nd1—O2—C1	49.2 (2)	C20—C19—O9—C18	1.8 (6)
O4—Nd1—O2—C1	−114.0 (4)	C17—C18—O9—C19	161.7 (4)

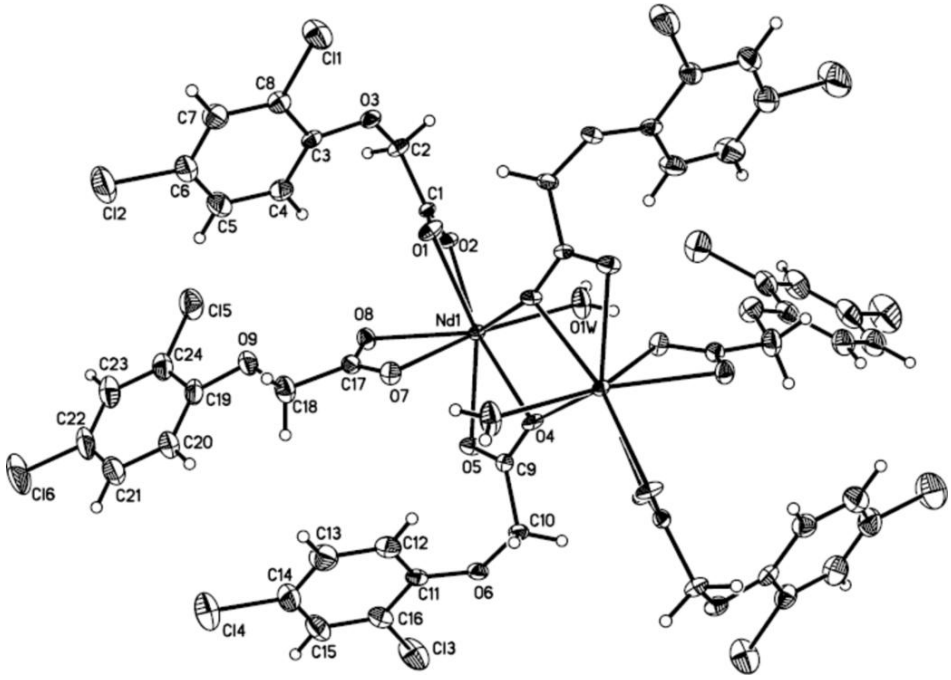
Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) *x*, −*y*+1/2, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W···O8^{i}	0.811 (19)	1.98 (3)	2.702 (4)	148 (4)
O1W—H2W···Cl5^{i}	0.807 (19)	2.89 (4)	3.422 (4)	125 (4)
O1W—H2W···O7^{ii}	0.807 (19)	2.66 (2)	3.395 (5)	152 (4)

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) *x*, −*y*+1/2, *z*−1/2.

Fig. 1


Cl1
C8
C7
O3
C3
C2
C1
C6
Cl2
C5
C4
O1
O2
Cl5
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Nd1
O1W
C24
O9
C23
C19
C17
O7
C18
C22
C20
O4
O5
C9
Cl6
C21
C10
C13
C12
C14
C11
O6
C16
Cl4
C15
Cl3

Fig. 2