

Di- μ -acetato-bis[triaquabis(thiocyanato- κ N)(pyridine *N*-oxide- κ O)neodymium(III)]

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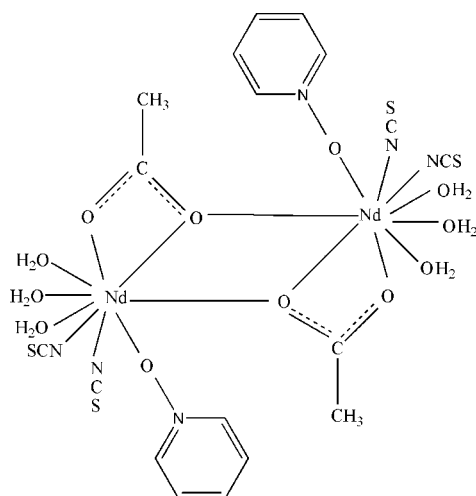
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.031; wR factor = 0.071; data-to-parameter ratio = 15.2.

The title binuclear complex, $[\text{Nd}_2(\mu\text{-C}_2\text{H}_3\text{O}_2)_2(\text{NCS})_4(\text{C}_5\text{H}_5\text{NO})_2(\text{H}_2\text{O})_6]$, lies about an inversion centre at the centroid of the four-membered Nd_2O_2 ring, with the two acetate ions acting as bridging ligands. A monodentate pyridine *N*-oxide ligand, two terminal thiocyanate groups and three water molecules complete the coordination environments of each nine-coordinate Nd^{III} atom. $\text{O}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{N}$ and $\text{O}-\text{H}\cdots\text{S}$ hydrogen bonds link the molecules into a three-dimensional network.

Related literature

For related structures, see: Kato *et al.* (1964); Zhang *et al.* (2006).



Experimental

Crystal data

$[\text{Nd}_2(\text{C}_2\text{H}_3\text{O}_2)_2(\text{NCS})_4(\text{C}_5\text{H}_5\text{NO})_2(\text{H}_2\text{O})_6]$
 $M_r = 937.18$
 Monoclinic, $P2_1/n$
 $a = 9.1588$ (15) Å
 $b = 16.185$ (3) Å
 $c = 11.3892$ (18) Å

$\beta = 102.813$ (2)°
 $V = 1646.3$ (5) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 3.43$ mm⁻¹
 $T = 298$ (2) K
 $0.56 \times 0.07 \times 0.06$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.249$, $T_{\text{max}} = 0.821$

6827 measured reflections
 2900 independent reflections
 2545 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.071$
 $S = 1.02$
 2900 reflections
 191 parameters

9 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.39$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.95$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O4}-\text{H6}\cdots\text{O1}^{\text{i}}$	0.85	1.83	2.675 (5)	178
$\text{O6}-\text{H9}\cdots\text{O2}^{\text{ii}}$	0.85	1.85	2.686 (4)	167
$\text{O6}-\text{H8}\cdots\text{S2}^{\text{iii}}$	0.85	2.31	3.162 (4)	175
$\text{O5}-\text{H10}\cdots\text{S2}^{\text{iii}}$	0.85	2.73	3.534 (4)	159
$\text{O5}-\text{H11}\cdots\text{S1}^{\text{iv}}$	0.84	2.40	3.236 (4)	169
$\text{O4}-\text{H7}\cdots\text{S1}^{\text{ii}}$	0.82	2.45	3.220 (4)	157
$\text{O4}-\text{H6}\cdots\text{N1}^{\text{i}}$	0.85	2.70	3.484 (5)	155

Symmetry codes: (i) $-x + 2, -y + 2, -z + 1$; (ii) $-x + 1, -y + 2, -z + 1$; (iii) $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (iv) $x + \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2001); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; 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: SJ2319).

References

- Bruker (1997). SMART (Version 5.6) and SAINT (Version 5.06a), Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2001). SHELXTL. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
 Kato, M., Jonassen, H. B. & Fanning, J. C. (1964). *Chem. Rev.* **64**, 99–128.
 Sheldrick, G. M. (1996). SADABS. Version 2.10. University of Göttingen, Germany.
 Zhang, S.-G., Li, W.-N. & Shi, J.-M. (2006). *Acta Cryst.* **E62**, m3398–m3400.

supplementary materials

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Comment

Acetate, thiocyanate and pyridine *N*-oxide or its derivatives are all known to function as bridging ligands (Kato *et al.*, 1964; Zhang *et al.*, 2006), and we are interested in complexes with mixed bridge ligands which led to the synthesis of the title complex (I) and we report its structure here, Fig. 1. In the binuclear structure acetate acts as a bridging ligand, whereas thiocyanate, water and pyridine *N*-oxide only function as terminal ligands. The Nd and bridging acetate O atoms form a four-membered ring by virtue of the crystallographic inversion center which is at the centroid of the ring. The distance between the bridged Nd(III) ions is 4.4167 (7) Å, and atoms Nd1, Nd1ⁱ, O3 and O3ⁱ are strictly coplanar (*i* = $-x + 2, -y + 2, -z + 1$). An extensive set of O—H \cdots O, O—H \cdots N and O—H \cdots S hydrogen bonds (Table 1) connect the binuclear units into a three-dimensional supermolecular structure.

Experimental

Nd(ClO₄)₃·6H₂O (0.2891 g, 0.525 mmol), NaSCN (0.0872 g, 1.08 mmol), pyridine *N*-oxide (0.0502 g, 0.528 mmol) and Na(CH₃COO) (0.0435 g, 0.530 mmol) were each dissolved in 5 ml of water. The solutions were then mixed together and stirred for a few minutes. Colourless transparent single crystals were obtained on allowing the solution to stand for two weeks at room temperature.

Refinement

The H atoms from H₂O were found in a difference Fourier map and fixed with $d(\text{O—H}) = 0.8200\text{--}0.8502$ Å, $U_{\text{iso}}(\text{H}) = 1.5_{\text{eq}}(\text{O})$. Other H atoms were placed in calculated positions, and refined as riding, with $\text{C—H} = 0.93$ Å, $U_{\text{iso}}(\text{H}) = 1.2_{\text{eq}}(\text{C})$ for the pyridine ring; $\text{C—H} = 0.96$ Å, $U_{\text{iso}}(\text{H}) = 1.5_{\text{eq}}(\text{C})$ for the methyl groups.

Figures

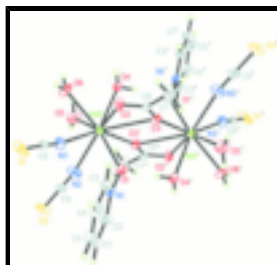


Fig. 1. Binuclear structure of (I) showing the atom numbering scheme with thermal ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) $-x + 2, -y + 2, -z + 1$].

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Crystal data

$[\text{Nd}_2(\text{C}_2\text{H}_3\text{O}_2)_2(\text{NCS})_4(\text{C}_5\text{H}_5\text{NO})_2(\text{H}_2\text{O})_6]$	$F_{000} = 916$
$M_r = 937.18$	$D_x = 1.891 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: -P 2yn	$\lambda = 0.71073 \text{ \AA}$
$a = 9.1588 (15) \text{ \AA}$	Cell parameters from 3146 reflections
$b = 16.185 (3) \text{ \AA}$	$\theta = 2.2\text{--}26.8^\circ$
$c = 11.3892 (18) \text{ \AA}$	$\mu = 3.43 \text{ mm}^{-1}$
$\beta = 102.813 (2)^\circ$	$T = 298 (2) \text{ K}$
$V = 1646.3 (5) \text{ \AA}^3$	Prism, colourless
$Z = 2$	$0.56 \times 0.07 \times 0.06 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2900 independent reflections
Radiation source: fine-focus sealed tube	2545 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.029$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.2^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{\text{min}} = 0.249$, $T_{\text{max}} = 0.821$	$k = -19 \rightarrow 17$
6827 measured reflections	$l = -13 \rightarrow 13$

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-atom parameters constrained
$wR(F^2) = 0.071$	$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 1.869P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
2900 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
191 parameters	$\Delta\rho_{\text{max}} = 1.39 \text{ e \AA}^{-3}$
9 restraints	$\Delta\rho_{\text{min}} = -0.95 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Nd1	0.81351 (3)	0.914089 (14)	0.50289 (2)	0.02859 (10)
S2	0.9773 (2)	0.60651 (9)	0.60836 (14)	0.0636 (5)
S1	0.4319 (2)	0.85963 (10)	0.77853 (17)	0.0731 (5)
C6	0.8144 (5)	1.0972 (3)	0.5558 (4)	0.0324 (11)
O3	0.9353 (3)	1.07210 (19)	0.5326 (3)	0.0367 (8)
N1	0.9405 (4)	0.9164 (2)	0.8172 (3)	0.0355 (9)
O6	0.5523 (4)	0.9109 (2)	0.3919 (3)	0.0516 (10)
H9	0.4761	0.9210	0.4205	0.077*
H8	0.5265	0.9077	0.3156	0.077*
O1	0.9538 (4)	0.9411 (2)	0.7079 (3)	0.0465 (9)
O2	0.7084 (3)	1.0477 (2)	0.5525 (3)	0.0384 (8)
O5	0.7805 (5)	0.8141 (2)	0.3268 (3)	0.0626 (11)
H10	0.7260	0.8323	0.2620	0.094*
H11	0.8307	0.7728	0.3133	0.094*
N3	0.6407 (5)	0.8676 (3)	0.6364 (4)	0.0471 (11)
N2	0.9058 (6)	0.7726 (3)	0.5737 (5)	0.0645 (14)
C9	0.9357 (6)	0.7034 (4)	0.5892 (4)	0.0447 (13)
C2	1.0314 (6)	0.8571 (3)	0.8735 (5)	0.0514 (14)
H2	1.0996	0.8315	0.8358	0.062*
C7	0.7971 (7)	1.1846 (4)	0.5870 (7)	0.076 (2)
H7A	0.6963	1.1942	0.5948	0.114*
H7B	0.8186	1.2194	0.5246	0.114*
H7C	0.8653	1.1972	0.6618	0.114*
C1	1.0225 (7)	0.8348 (4)	0.9877 (6)	0.0655 (18)
H1	1.0855	0.7939	1.0281	0.079*
O4	0.7882 (4)	0.9858 (2)	0.3048 (3)	0.0408 (8)
H7	0.7158	1.0170	0.2940	0.061*
H6	0.8692	1.0094	0.2993	0.061*
C3	0.8400 (6)	0.9531 (3)	0.8683 (5)	0.0438 (12)
H3	0.7771	0.9936	0.8268	0.053*
C4	0.8298 (7)	0.9311 (4)	0.9810 (5)	0.0622 (18)
H4	0.7595	0.9565	1.0167	0.075*
C5	0.9224 (8)	0.8719 (5)	1.0422 (6)	0.077 (2)

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H5	0.9169	0.8571	1.1200	0.092*
C8	0.5514 (5)	0.8627 (3)	0.6923 (4)	0.0358 (11)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.02128 (15)	0.03128 (15)	0.03543 (16)	0.00006 (10)	0.01103 (11)	0.00093 (11)
S2	0.0951 (13)	0.0463 (9)	0.0496 (9)	0.0206 (8)	0.0162 (9)	0.0095 (7)
S1	0.0744 (12)	0.0619 (10)	0.1033 (13)	0.0212 (8)	0.0629 (11)	0.0405 (10)
C6	0.023 (3)	0.032 (3)	0.044 (3)	0.0065 (19)	0.012 (2)	-0.003 (2)
O3	0.0235 (17)	0.0415 (19)	0.048 (2)	0.0027 (14)	0.0133 (15)	0.0014 (15)
N1	0.030 (2)	0.041 (2)	0.035 (2)	-0.0081 (18)	0.0058 (18)	0.0038 (18)
O6	0.0186 (17)	0.090 (3)	0.048 (2)	-0.0006 (17)	0.0123 (16)	-0.013 (2)
O1	0.037 (2)	0.070 (2)	0.0341 (18)	-0.0149 (18)	0.0091 (16)	0.0106 (17)
O2	0.0251 (18)	0.0377 (19)	0.057 (2)	-0.0008 (15)	0.0186 (16)	-0.0071 (16)
O5	0.072 (3)	0.051 (2)	0.059 (2)	0.020 (2)	0.002 (2)	-0.015 (2)
N3	0.041 (3)	0.054 (3)	0.049 (3)	-0.005 (2)	0.015 (2)	0.008 (2)
N2	0.075 (4)	0.051 (3)	0.072 (3)	0.018 (3)	0.026 (3)	0.020 (3)
C9	0.043 (3)	0.055 (4)	0.037 (3)	0.007 (3)	0.009 (2)	0.009 (3)
C2	0.045 (3)	0.049 (3)	0.061 (4)	0.007 (3)	0.013 (3)	0.007 (3)
C7	0.049 (4)	0.043 (4)	0.144 (7)	-0.008 (3)	0.036 (4)	-0.025 (4)
C1	0.062 (4)	0.064 (4)	0.063 (4)	-0.005 (3)	-0.003 (3)	0.026 (3)
O4	0.0265 (18)	0.048 (2)	0.048 (2)	-0.0047 (15)	0.0069 (15)	0.0086 (16)
C3	0.033 (3)	0.049 (3)	0.050 (3)	-0.001 (2)	0.010 (2)	-0.004 (3)
C4	0.052 (4)	0.092 (5)	0.049 (4)	-0.014 (3)	0.025 (3)	-0.013 (3)
C5	0.075 (5)	0.110 (6)	0.046 (4)	-0.032 (5)	0.017 (4)	0.016 (4)
C8	0.035 (3)	0.037 (3)	0.036 (3)	-0.002 (2)	0.010 (2)	0.007 (2)

Geometric parameters (\AA , $^\circ$)

Nd1—O3 ⁱ	2.433 (3)	O6—H8	0.8502
Nd1—O1	2.441 (3)	O5—H10	0.8473
Nd1—O6	2.446 (3)	O5—H11	0.8439
Nd1—O2	2.483 (3)	N3—C8	1.145 (6)
Nd1—O4	2.502 (3)	N2—C9	1.157 (7)
Nd1—N2	2.511 (5)	C2—C1	1.369 (8)
Nd1—N3	2.540 (4)	C2—H2	0.9300
Nd1—O5	2.542 (4)	C7—H7A	0.9600
Nd1—O3	2.781 (3)	C7—H7B	0.9600
S2—C9	1.617 (6)	C7—H7C	0.9600
S1—C8	1.626 (5)	C1—C5	1.357 (10)
C6—O2	1.253 (5)	C1—H1	0.9300
C6—O3	1.261 (5)	O4—H7	0.8200
C6—C7	1.476 (7)	O4—H6	0.8492
O3—Nd1 ⁱ	2.433 (3)	C3—C4	1.354 (8)
N1—C3	1.333 (6)	C3—H3	0.9300
N1—C2	1.338 (6)	C4—C5	1.365 (10)
N1—O1	1.339 (5)	C4—H4	0.9300

O6—H9	0.8483	C5—H5	0.9300
O3 ⁱ —Nd1—O1	79.97 (11)	Nd1 ⁱ —O3—Nd1	115.65 (11)
O3 ⁱ —Nd1—O6	140.26 (11)	C3—N1—C2	121.8 (5)
O1—Nd1—O6	138.13 (12)	C3—N1—O1	119.2 (4)
O3 ⁱ —Nd1—O2	112.74 (10)	C2—N1—O1	119.0 (4)
O1—Nd1—O2	76.98 (12)	Nd1—O6—H9	126.2
O6—Nd1—O2	75.61 (11)	Nd1—O6—H8	123.2
O3 ⁱ —Nd1—O4	73.13 (10)	H9—O6—H8	109.8
O1—Nd1—O4	134.66 (11)	N1—O1—Nd1	134.3 (3)
O6—Nd1—O4	70.08 (11)	C6—O2—Nd1	103.1 (3)
O2—Nd1—O4	80.67 (11)	Nd1—O5—H10	114.2
O3 ⁱ —Nd1—N2	82.75 (14)	Nd1—O5—H11	132.3
O1—Nd1—N2	77.77 (15)	H10—O5—H11	110.8
O6—Nd1—N2	111.58 (16)	C8—N3—Nd1	165.9 (4)
O2—Nd1—N2	147.25 (14)	C9—N2—Nd1	169.4 (5)
O4—Nd1—N2	132.08 (14)	N2—C9—S2	179.0 (5)
O3 ⁱ —Nd1—N3	149.81 (12)	N1—C2—C1	118.9 (6)
O1—Nd1—N3	75.30 (12)	N1—C2—H2	120.5
O6—Nd1—N3	68.60 (13)	C1—C2—H2	120.5
O2—Nd1—N3	78.31 (13)	C6—C7—H7A	109.5
O4—Nd1—N3	137.05 (12)	C6—C7—H7B	109.5
N2—Nd1—N3	75.37 (16)	H7A—C7—H7B	109.5
O3 ⁱ —Nd1—O5	83.04 (12)	C6—C7—H7C	109.5
O1—Nd1—O5	144.44 (13)	H7A—C7—H7C	109.5
O6—Nd1—O5	69.37 (12)	H7B—C7—H7C	109.5
O2—Nd1—O5	138.57 (12)	C5—C1—C2	120.5 (6)
O4—Nd1—O5	67.24 (12)	C5—C1—H1	119.8
N2—Nd1—O5	69.24 (15)	C2—C1—H1	119.8
N3—Nd1—O5	107.62 (14)	Nd1—O4—H7	109.4
O3 ⁱ —Nd1—O3	64.35 (12)	Nd1—O4—H6	111.6
O1—Nd1—O3	66.88 (11)	H7—O4—H6	113.8
O6—Nd1—O3	113.70 (11)	N1—C3—C4	119.8 (6)
O2—Nd1—O3	48.43 (10)	N1—C3—H3	120.1
O4—Nd1—O3	68.72 (10)	C4—C3—H3	120.1
N2—Nd1—O3	134.63 (15)	C3—C4—C5	120.2 (6)
N3—Nd1—O3	119.09 (12)	C3—C4—H4	119.9
O5—Nd1—O3	130.97 (12)	C5—C4—H4	119.9
O2—C6—O3	119.9 (4)	C1—C5—C4	118.9 (6)
O2—C6—C7	119.8 (4)	C1—C5—H5	120.6
O3—C6—C7	120.3 (4)	C4—C5—H5	120.6
C6—O3—Nd1 ⁱ	155.7 (3)	N3—C8—S1	176.2 (5)
C6—O3—Nd1	88.6 (3)		
O2—C6—O3—Nd1 ⁱ	174.7 (5)	O1—Nd1—O2—C6	69.5 (3)
C7—C6—O3—Nd1 ⁱ	-5.3 (11)	O6—Nd1—O2—C6	-142.5 (3)
O2—C6—O3—Nd1	-1.7 (4)	O4—Nd1—O2—C6	-70.8 (3)
C7—C6—O3—Nd1	178.4 (5)	N2—Nd1—O2—C6	109.9 (4)

supplementary materials

O3 ⁱ —Nd1—O3—C6	178.3 (3)	N3—Nd1—O2—C6	146.9 (3)
O1—Nd1—O3—C6	-92.0 (3)	O5—Nd1—O2—C6	-109.6 (3)
O6—Nd1—O3—C6	42.2 (3)	O3—Nd1—O2—C6	-1.0 (3)
O2—Nd1—O3—C6	1.0 (3)	O3 ⁱ —Nd1—N3—C8	129.8 (16)
O4—Nd1—O3—C6	97.5 (3)	O1—Nd1—N3—C8	93.8 (16)
N2—Nd1—O3—C6	-133.8 (3)	O6—Nd1—N3—C8	-64.6 (16)
N3—Nd1—O3—C6	-35.6 (3)	O2—Nd1—N3—C8	14.4 (16)
O5—Nd1—O3—C6	124.8 (3)	O4—Nd1—N3—C8	-47.9 (17)
O3 ⁱ —Nd1—O3—Nd1 ⁱ	0.0	N2—Nd1—N3—C8	174.7 (17)
O1—Nd1—O3—Nd1 ⁱ	89.71 (15)	O5—Nd1—N3—C8	-123.1 (16)
O6—Nd1—O3—Nd1 ⁱ	-136.12 (13)	O3—Nd1—N3—C8	41.5 (17)
O2—Nd1—O3—Nd1 ⁱ	-177.4 (2)	O3 ⁱ —Nd1—N2—C9	-102 (3)
O4—Nd1—O3—Nd1 ⁱ	-80.88 (14)	O1—Nd1—N2—C9	177 (3)
N2—Nd1—O3—Nd1 ⁱ	47.9 (2)	O6—Nd1—N2—C9	40 (3)
N3—Nd1—O3—Nd1 ⁱ	146.10 (14)	O2—Nd1—N2—C9	137 (3)
O5—Nd1—O3—Nd1 ⁱ	-53.50 (19)	O4—Nd1—N2—C9	-42 (3)
C3—N1—O1—Nd1	-79.8 (5)	N3—Nd1—N2—C9	99 (3)
C2—N1—O1—Nd1	102.1 (5)	O5—Nd1—N2—C9	-17 (3)
O3 ⁱ —Nd1—O1—N1	-146.6 (4)	O3—Nd1—N2—C9	-144 (3)
O6—Nd1—O1—N1	46.9 (5)	Nd1—N2—C9—S2	30 (34)
O2—Nd1—O1—N1	97.1 (4)	C3—N1—C2—C1	-1.2 (8)
O4—Nd1—O1—N1	159.5 (4)	O1—N1—C2—C1	176.9 (5)
N2—Nd1—O1—N1	-61.9 (4)	N1—C2—C1—C5	0.4 (9)
N3—Nd1—O1—N1	16.0 (4)	C2—N1—C3—C4	0.9 (8)
O5—Nd1—O1—N1	-83.9 (5)	O1—N1—C3—C4	-177.2 (5)
O3—Nd1—O1—N1	147.2 (4)	N1—C3—C4—C5	0.2 (9)
O3—C6—O2—Nd1	1.9 (5)	C2—C1—C5—C4	0.7 (10)
C7—C6—O2—Nd1	-178.1 (5)	C3—C4—C5—C1	-1.0 (10)
O3 ⁱ —Nd1—O2—C6	-3.6 (3)	Nd1—N3—C8—S1	-75 (8)

Symmetry codes: (i) $-x+2, -y+2, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H6 \cdots O1 ⁱ	0.85	1.83	2.675 (5)	178
O6—H9 \cdots O2 ⁱⁱ	0.85	1.85	2.686 (4)	167
O6—H8 \cdots S2 ⁱⁱⁱ	0.85	2.31	3.162 (4)	175
O5—H10 \cdots S2 ⁱⁱⁱ	0.85	2.73	3.534 (4)	159
O5—H11 \cdots S1 ^{iv}	0.84	2.40	3.236 (4)	169
O4—H7 \cdots S1 ⁱⁱ	0.82	2.45	3.220 (4)	157
O4—H6 \cdots N1 ⁱ	0.85	2.70	3.484 (5)	155

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $-x+1, -y+2, -z+1$; (iii) $x-1/2, -y+3/2, z-1/2$; (iv) $x+1/2, -y+3/2, z-1/2$.

Fig. 1

