Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetrakis(μ-propanoato-κ²O:O′)-bis[(1,10-phenanthroline-κ²N,N′)-(propanoato-κ²O,O′)samarium(III)]

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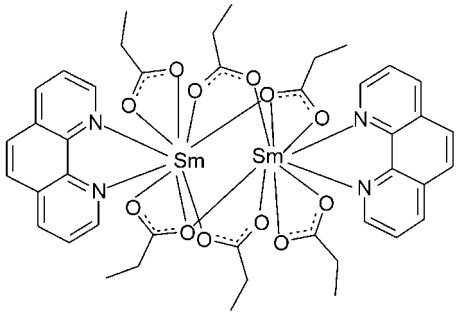
Received 9 November 2007; accepted 30 November 2007

Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.004 Å; R factor = 0.021; wR factor = 0.064; data-to-parameter ratio = 16.9.

The title complex, $[Sm_2(C_3H_5O_2)_6(C_{12}H_8N_2)_2]$, is a dinuclear centrosymmetric molecule, in which two crystallographically equivalent Sm atoms, separated by 3.9502 (2) Å, are bridged by four propanoate anions. Each Sm atom is coordinated by two N atoms from one chelating phenanthroline ligand and seven carboxylate O atoms from five propanoate anions, to form a distorted tricapped trigonal prism.

Related literature

For related literature, see: Lu *et al.* (2000); Lu, Lu, Wu & Wang (2001); Lu, Wu & Wang (2001); Wang *et al.* (2005).



Experimental

Crystal data

$[Sm_2(C_3H_5O_2)_6(C_{12}H_8N_2)_2]$
M_r = 1099.55
Monoclinic, $P2_1/n$
a = 9.5740 (2) Å
b = 18.3182 (5) Å
c = 12.7307 (3) Å
β = 107.103 (1)°
V = 2133.95 (9) Å³
Z = 2
Mo $K\alpha$ radiation
μ = 2.79 mm⁻¹
T = 290 (2) K
0.25 × 0.21 × 0.17 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.508, T_{max} = 0.613
22209 measured reflections
5133 independent reflections
4563 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.065
S = 0.96
5133 reflections
275 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.10 e Å⁻³
$\Delta\rho_{min}$ = −0.66 e Å⁻³

Table 1
Selected bond lengths (Å).

Sm1—O1	2.5901 (16)	Sm1—O5	2.4030 (16)
Sm1—O2	2.5432 (15)	Sm1—O6^{i}	2.4023 (15)
Sm1—O2^{i}	2.3783 (14)	Sm1—N1	2.6528 (19)
Sm1—O3	2.5078 (19)	Sm1—N2	2.6042 (16)
Sm1—O4	2.4608 (17)	Sm1···Sm1^{i}	3.9502 (2)

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

Data collection: *APEX2* (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*.

This work was supported by Jiangxi Provincial Natural Science Foundation (grant No. 0620018) and Jiangxi University of Science and Technology Doctoral Foundation (grant No. 2003-1).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2147).

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supplementary materials

Acta Cryst. (2008). E**64**, m102 [**doi:10.1107/S1600536807064720**]

Tetrakis(μ-propanoato-κ^2O:O')bis[(1,10-phenanthroline-κ^2N,N')(propanoato-κ^2O,O')samarium(III)]

C.-X. Wang, Z.-F. Li, S.-H. Xiong and P. Wang

Comment

In the recent years, a series of dimeric $[M(\text{phen})(C_5H_7O_2)_3]_2$ (M= La (Lu, Lu, Wu & Wang, 2001; Lu, Wu & Wang, 2001), Tb, Ho (Lu *et al.*, 2000), Dy (Wang *et al.*, 2005), $C_5H_7O_2$= *trans*-2,3-dimethylacrylate) analogues have been reported, in which the lanthanide ions form a dinuclear centrosymmetric molecule through the coordination of bridging carboxylato groups. An isostructural complex, $[Sm(\text{phen})(C_3H_5O_2)_3]_2$, (I), was obtained after the *trans*-2,3-dimethylacrylate ligands were replaced by propanoato ligands. Each Sm atom exhibits a distorted tricapped trigonal prism coordinated by two N atoms from one chelating phenanthroline ligand and seven carboxyl oxygen atoms from five propanoato anions (Fig. 1). The carboxylato groups exhibit three different coordination modes: a common bidentate chelating mode, a bidentate bridging mode, and tridentate bridging mode, resulting in a dinuclear centrosymmetric molecule with the Sm1···Sm1^{i} distance of 3.9502 (2) Å. The Sm1—O bond distances vary from 2.3784 (14)Å to 2.5901 (16)Å and the Sm1—N bond length are 2.6042 (16)Å and 2.6528 (19)Å (Table 1) similar to those found in the previously mentioned *trans*-2,3-dimethylacrylato complexes. The C—O and C—C distances are within the range of 1.242 (3)Å to 1.272 (3)Å and 1.502 (4) Å–1.515 (3) Å, respectively. The dimeric molecules are assembled into two-dimensional sheets parallel to (100) by face-to-face π-π stacking interactions. The phenanthroline rings involved in π-π stacking interactions located at (x, y, z) and (1 - x, 1 - y, 2 - z) are strictly parallel with an interplanar spacing of 3.301 (3)Å [the centroid separation of 4.492 (2) Å and the centroid offset of 3.047 (3) Å] and those located at (x, y, z) and (2 - x, 1 - y, 2 - z) with interplanar spacing of 3.371 (3) Å [the centroid separation of 4.838 (3) Å and the centroid offset of 3.470 (3) Å]. However, there are no direction-specific interactions between adjacent sheets.

Experimental

A solution obtained by dissolving 0.200 g (0.463 mmol) of Sm_2O_3 in 20 ml (36.5%) HCl was evaporated to dryness. Then 25 ml of CH_3OH / H_2O (1:1 *v*/*v*) was added followed by 0.5 ml of propanoic acid, and 0.25 g (1.261 mmol) phenanthroline with strring. A colourless solution was left for several days and crystals were obtain by slow evaporation at room temperature. Yield of 20% based on the initial Sm_2O_3.

Refinement

H atoms attached to C atoms were included at calculated positions and treated as riding atoms, with C–H distances of 0.93 Å (aromatic), 0.97 Å (methylene) and 0.96 Å (methyl), and with U_{iso}(H) values of 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq} for others.

Figures

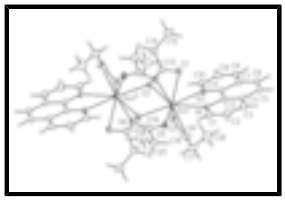


Fig. 1. The dinuclear structure of the title compound with the atom numbering scheme showing displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) 1 - *x*, 1 - *y*, 1 - *z*.]

Tetrakis(μ-propanoato-κ^2*O*:*O*')bis[(1,10-phenanthroline- κ^2*N*,*N*')(propanoato-κ^2*O*,*O*')samarium(III)]

Crystal data

$[Sm_2(C_3H_5O_2)_6(C_{12}H_8N_2)_2]$	F_{000} = 1092
M_r = 1099.55	D_x = 1.711 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 198 reflections
a = 9.5740 (2) Å	θ = 2.1–26.7º
b = 18.3182 (5) Å	μ = 2.79 mm^{-1}
c = 12.7307 (3) Å	*T* = 290 (2) K
β = 107.103 (1)º	Cloumn, colourless
V = 2133.95 (9) Å^3	0.25 × 0.21 × 0.17 mm
Z = 2	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	5133 independent reflections
Radiation source: fine-focus sealed tube	4563 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
T = 290(2) K	θ_{max} = 28.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	*h* = −11→12
T_{min} = 0.508, T_{max} = 0.613	*k* = −24→22
22209 measured reflections	*l* = −16→16

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.022	$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.065	$(\Delta/\sigma)_{max}$ = 0.012
S = 0.96	$\Delta\rho_{max}$ = 1.10 e Å^{-3}

5133 reflections

275 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$\Delta\rho_{min} = -0.66$ e Å^{-3}

Extinction correction: SHELXL, $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00050 (8)

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}
Sm1	0.603212 (11)	0.530844 (5)	0.651651 (8)	0.0277 (6)
C1	0.8823 (3)	0.41499 (14)	0.8116 (2)	0.0425 (5)
H1	0.8910	0.4065	0.7418	0.051*
C2	0.9724 (3)	0.37486 (16)	0.9002 (2)	0.0532 (6)
H2	1.0371	0.3400	0.8887	0.064*
C3	0.9625 (3)	0.38827 (16)	1.0030 (2)	0.0523 (7)
H3	1.0208	0.3624	1.0627	0.063*
C4	0.8639 (2)	0.44146 (14)	1.01906 (18)	0.0403 (5)
C5	0.8517 (3)	0.45852 (16)	1.1256 (2)	0.0507 (7)
H5	0.9114	0.4349	1.1872	0.061*
C6	0.7545 (3)	0.50857 (16)	1.13715 (19)	0.0490 (6)
H6	0.7460	0.5183	1.2067	0.059*
C7	0.6635 (3)	0.54731 (14)	1.04381 (18)	0.0397 (5)
C8	0.5635 (3)	0.60054 (14)	1.05310 (19)	0.0450 (6)
H8	0.5534	0.6123	1.1216	0.054*
C9	0.4809 (3)	0.63520 (14)	0.96118 (19)	0.0456 (6)
H9	0.4151	0.6714	0.9663	0.055*
C10	0.4962 (3)	0.61560 (13)	0.85904 (18)	0.0400 (5)
H10	0.4383	0.6392	0.7967	0.048*
C11	0.6732 (3)	0.53143 (11)	0.93823 (18)	0.0333 (5)
C12	0.7774 (3)	0.47707 (11)	0.92520 (19)	0.0336 (5)
C13	0.4212 (2)	0.39864 (12)	0.61132 (16)	0.0322 (4)
C14	0.3063 (3)	0.33972 (16)	0.5805 (2)	0.0504 (6)
H14A	0.3459	0.2986	0.5505	0.060*
H14B	0.2234	0.3582	0.5230	0.060*
C15	0.2530 (4)	0.31277 (19)	0.6741 (2)	0.0685 (9)
H15A	0.3328	0.2911	0.7295	0.103*

H15B	0.1775	0.2771	0.6471	0.103*
H15C	0.2147	0.3531	0.7053	0.103*
C16	0.7414 (3)	0.66842 (13)	0.70839 (18)	0.0383 (5)
C17	0.8162 (3)	0.73884 (15)	0.7554 (3)	0.0549 (6)
H17A	0.7935	0.7762	0.6990	0.066*
H17B	0.9212	0.7316	0.7788	0.066*
C18	0.7672 (4)	0.76422 (16)	0.8528 (3)	0.0689 (9)
H18A	0.6629	0.7699	0.8304	0.103*
H18B	0.8126	0.8101	0.8790	0.103*
H18C	0.7951	0.7286	0.9106	0.103*
C19	0.7591 (2)	0.43839 (13)	0.47916 (17)	0.0352 (4)
C20	0.8978 (3)	0.40185 (17)	0.4716 (2)	0.0580 (7)
H20A	0.9536	0.4370	0.4435	0.070*
H20B	0.9561	0.3884	0.5451	0.070*
C21	0.8744 (4)	0.33504 (18)	0.4002 (3)	0.0666 (8)
H21A	0.8227	0.2989	0.4288	0.100*
H21B	0.9673	0.3157	0.3993	0.100*
H21C	0.8183	0.3478	0.3267	0.100*
N1	0.7860 (2)	0.46400 (9)	0.82208 (16)	0.0342 (4)
N2	0.58902 (19)	0.56515 (10)	0.84676 (13)	0.0328 (4)
O1	0.47819 (18)	0.41818 (9)	0.70787 (12)	0.0412 (4)
O2	0.45959 (17)	0.42819 (8)	0.53367 (11)	0.0349 (3)
O3	0.60502 (17)	0.66725 (10)	0.66879 (13)	0.0425 (4)
O4	0.81734 (19)	0.61156 (9)	0.71259 (15)	0.0451 (4)
O5	0.76476 (19)	0.46719 (8)	0.57009 (14)	0.0420 (4)
O6	0.65199 (16)	0.43918 (10)	0.39479 (12)	0.0394 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.0318 (9)	0.0357 (10)	0.0182 (9)	0.0015 (8)	0.0047 (7)	−0.0013 (7)
C1	0.0376 (13)	0.0473 (14)	0.0390 (13)	0.0044 (10)	0.0057 (10)	0.0005 (10)
C2	0.0483 (15)	0.0514 (15)	0.0538 (16)	0.0129 (12)	0.0052 (12)	0.0059 (12)
C3	0.0423 (14)	0.0595 (17)	0.0467 (15)	0.0055 (12)	−0.0008 (12)	0.0160 (12)
C4	0.0334 (12)	0.0507 (14)	0.0320 (12)	−0.0082 (11)	0.0012 (9)	0.0075 (10)
C5	0.0460 (16)	0.0687 (18)	0.0288 (13)	−0.0083 (13)	−0.0022 (11)	0.0131 (11)
C6	0.0552 (16)	0.0669 (17)	0.0224 (11)	−0.0122 (14)	0.0071 (11)	0.0029 (11)
C7	0.0441 (14)	0.0502 (13)	0.0233 (11)	−0.0129 (11)	0.0065 (10)	−0.0013 (9)
C8	0.0519 (15)	0.0567 (16)	0.0301 (12)	−0.0102 (12)	0.0181 (11)	−0.0074 (10)
C9	0.0527 (15)	0.0512 (15)	0.0387 (13)	−0.0032 (12)	0.0215 (11)	−0.0082 (10)
C10	0.0445 (13)	0.0473 (13)	0.0305 (11)	0.0021 (11)	0.0136 (10)	0.0001 (9)
C11	0.0335 (12)	0.0410 (13)	0.0240 (11)	−0.0098 (8)	0.0064 (9)	0.0003 (7)
C12	0.0291 (11)	0.0397 (13)	0.0274 (12)	−0.0080 (8)	0.0022 (9)	0.0023 (8)
C13	0.0329 (11)	0.0363 (12)	0.0272 (10)	0.0033 (9)	0.0081 (9)	0.0029 (8)
C14	0.0540 (16)	0.0587 (17)	0.0367 (13)	−0.0172 (13)	0.0092 (11)	−0.0020 (11)
C15	0.076 (2)	0.075 (2)	0.0565 (18)	−0.0412 (18)	0.0227 (16)	−0.0012 (15)
C16	0.0424 (13)	0.0419 (13)	0.0301 (11)	−0.0030 (10)	0.0102 (10)	0.0013 (9)
C17	0.0544 (16)	0.0416 (14)	0.0673 (18)	−0.0076 (12)	0.0153 (14)	−0.0041 (12)

C18	0.084 (2)	0.0476 (17)	0.071 (2)	−0.0055 (16)	0.0155 (17)	−0.0220 (14)
C19	0.0306 (11)	0.0443 (13)	0.0306 (11)	0.0030 (9)	0.0093 (9)	−0.0034 (9)
C20	0.0359 (14)	0.081 (2)	0.0528 (16)	0.0165 (13)	0.0068 (12)	−0.0200 (14)
C21	0.066 (2)	0.068 (2)	0.070 (2)	0.0218 (16)	0.0262 (16)	−0.0120 (15)
N1	0.0315 (10)	0.0411 (11)	0.0270 (10)	−0.0014 (7)	0.0031 (8)	−0.0005 (7)
N2	0.0341 (10)	0.0414 (11)	0.0230 (9)	−0.0014 (8)	0.0076 (7)	−0.0018 (7)
O1	0.0459 (10)	0.0540 (10)	0.0222 (7)	−0.0113 (8)	0.0076 (7)	0.0010 (6)
O2	0.0433 (10)	0.0396 (9)	0.0231 (10)	0.0012 (7)	0.0066 (6)	−0.0013 (6)
O3	0.0418 (10)	0.0357 (10)	0.0365 (9)	0.0029 (7)	0.0065 (7)	−0.0011 (8)
O4	0.0387 (9)	0.0404 (10)	0.0526 (11)	0.0004 (7)	0.0077 (8)	−0.0032 (7)
O5	0.0359 (10)	0.0584 (12)	0.0301 (9)	0.0114 (7)	0.0068 (7)	−0.0070 (6)
O6	0.0314 (8)	0.0551 (10)	0.0308 (8)	0.0058 (8)	0.0069 (7)	−0.0061 (7)

Geometric parameters (Å, °)

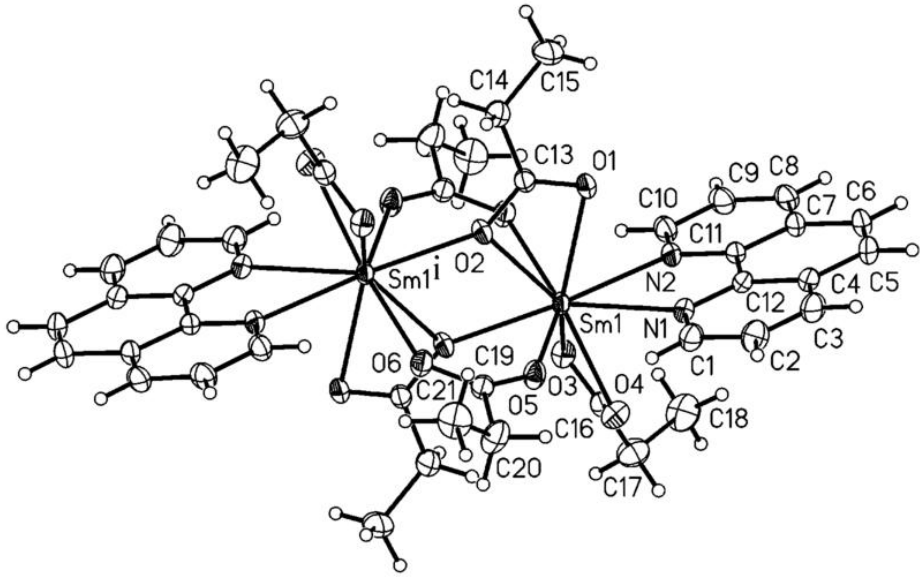
Sm1—O1	2.5901 (16)	C11—N2	1.355 (3)
Sm1—O2	2.5432 (15)	C11—C12	1.453 (3)
Sm1—O2^{i}	2.3783 (14)	C12—N1	1.361 (3)
Sm1—O3	2.5078 (19)	C13—O1	1.242 (3)
Sm1—O4	2.4608 (17)	C13—O2	1.272 (2)
Sm1—O5	2.4030 (16)	C13—C14	1.508 (3)
Sm1—O6^{i}	2.4023 (15)	C14—C15	1.511 (4)
Sm1—N1	2.6528 (19)	C14—H14A	0.9700
Sm1—N2	2.6042 (16)	C14—H14B	0.9700
Sm1—Sm1^{i}	3.9502 (2)	C15—H15A	0.9600
C1—N1	1.321 (3)	C15—H15B	0.9600
C1—C2	1.409 (4)	C15—H15C	0.9600
C1—H1	0.9300	C16—O3	1.254 (3)
C2—C3	1.362 (4)	C16—O4	1.262 (3)
C2—H2	0.9300	C16—C17	1.511 (3)
C3—C4	1.413 (4)	C17—C18	1.521 (4)
C3—H3	0.9300	C17—H17A	0.9700
C4—C12	1.399 (3)	C17—H17B	0.9700
C4—C5	1.430 (4)	C18—H18A	0.9600
C5—C6	1.345 (4)	C18—H18B	0.9600
C5—H5	0.9300	C18—H18C	0.9600
C6—C7	1.437 (3)	C19—O6	1.248 (3)
C6—H6	0.9300	C19—O5	1.259 (3)
C7—C8	1.396 (4)	C19—C20	1.515 (3)
C7—C11	1.405 (3)	C20—C21	1.502 (4)
C8—C9	1.361 (4)	C20—H20A	0.9700
C8—H8	0.9300	C20—H20B	0.9700
C9—C10	1.398 (3)	C21—H21A	0.9600
C9—H9	0.9300	C21—H21B	0.9600
C10—N2	1.323 (3)	C21—H21C	0.9600
C10—H10	0.9300		
O2^{i}—Sm1—O6^{i}	75.03 (5)	C8—C9—H9	120.4
O2^{i}—Sm1—O5	74.43 (6)	C10—C9—H9	120.4

O6^{i}—Sm1—O5	137.89 (5)	N2—C10—C9	123.2 (2)
O2^{i}—Sm1—O4	93.86 (6)	N2—C10—H10	118.4
O6^{i}—Sm1—O4	129.27 (6)	C9—C10—H10	118.4
O5—Sm1—O4	81.11 (6)	N2—C11—C7	122.5 (2)
O2^{i}—Sm1—O3	76.42 (5)	N2—C11—C12	117.99 (19)
O6^{i}—Sm1—O3	76.95 (6)	C7—C11—C12	119.5 (2)
O5—Sm1—O3	122.16 (6)	N1—C12—C4	123.6 (2)
O4—Sm1—O3	52.42 (5)	N1—C12—C11	118.0 (2)
O2^{i}—Sm1—O2	73.28 (5)	C4—C12—C11	118.4 (2)
O6^{i}—Sm1—O2	71.91 (5)	O1—C13—O2	120.2 (2)
O5—Sm1—O2	72.00 (5)	O1—C13—C14	122.54 (19)
O4—Sm1—O2	152.38 (5)	O2—C13—C14	117.24 (19)
O3—Sm1—O2	140.97 (5)	C13—C14—C15	114.8 (2)
O2^{i}—Sm1—O1	121.53 (5)	C13—C14—H14A	108.6
O6^{i}—Sm1—O1	74.39 (6)	C15—C14—H14A	108.6
O5—Sm1—O1	98.12 (5)	C13—C14—H14B	108.6
O4—Sm1—O1	143.28 (6)	C15—C14—H14B	108.6
O3—Sm1—O1	139.62 (5)	H14A—C14—H14B	107.6
O2—Sm1—O1	50.24 (4)	C14—C15—H15A	109.5
O2^{i}—Sm1—N2	143.24 (6)	C14—C15—H15B	109.5
O6^{i}—Sm1—N2	81.08 (5)	H15A—C15—H15B	109.5
O5—Sm1—N2	138.59 (6)	C14—C15—H15C	109.5
O4—Sm1—N2	80.02 (6)	H15A—C15—H15C	109.5
O3—Sm1—N2	71.19 (5)	H15B—C15—H15C	109.5
O2—Sm1—N2	124.81 (5)	O3—C16—O4	121.4 (2)
O1—Sm1—N2	76.74 (5)	O3—C16—C17	119.3 (2)
O2^{i}—Sm1—N1	150.52 (6)	O4—C16—C17	119.2 (2)
O6^{i}—Sm1—N1	133.27 (6)	C16—C17—C18	111.1 (2)
O5—Sm1—N1	77.04 (6)	C16—C17—H17A	109.4
O4—Sm1—N1	74.42 (6)	C18—C17—H17A	109.4
O3—Sm1—N1	113.75 (5)	C16—C17—H17B	109.4
O2—Sm1—N1	104.70 (5)	C18—C17—H17B	109.4
O1—Sm1—N1	69.73 (5)	H17A—C17—H17B	108.0
N2—Sm1—N1	62.50 (6)	C17—C18—H18A	109.5
O2^{i}—Sm1—Sm1^{i}	38.07 (4)	C17—C18—H18B	109.5
O6^{i}—Sm1—Sm1^{i}	69.18 (4)	H18A—C18—H18B	109.5
O5—Sm1—Sm1^{i}	68.86 (4)	C17—C18—H18C	109.5
O4—Sm1—Sm1^{i}	127.66 (4)	H18A—C18—H18C	109.5
O3—Sm1—Sm1^{i}	111.02 (4)	H18B—C18—H18C	109.5
O2—Sm1—Sm1^{i}	35.21 (3)	O6—C19—O5	126.0 (2)
O1—Sm1—Sm1^{i}	84.44 (3)	O6—C19—C20	117.7 (2)
N2—Sm1—Sm1^{i}	148.20 (4)	O5—C19—C20	116.3 (2)
N1—Sm1—Sm1^{i}	133.44 (4)	C21—C20—C19	114.9 (2)
N1—C1—C2	123.7 (3)	C21—C20—H20A	108.5

N1—C1—H1	118.2	C19—C20—H20A	108.5
C2—C1—H1	118.2	C21—C20—H20B	108.5
C3—C2—C1	118.4 (3)	C19—C20—H20B	108.5
C3—C2—H2	120.8	H20A—C20—H20B	107.5
C1—C2—H2	120.8	C20—C21—H21A	109.5
C2—C3—C4	120.1 (2)	C20—C21—H21B	109.5
C2—C3—H3	119.9	H21A—C21—H21B	109.5
C4—C3—H3	119.9	C20—C21—H21C	109.5
C12—C4—C3	116.8 (2)	H21A—C21—H21C	109.5
C12—C4—C5	121.0 (2)	H21B—C21—H21C	109.5
C3—C4—C5	122.2 (2)	C1—N1—C12	117.4 (2)
C6—C5—C4	120.3 (2)	C1—N1—Sm1	122.88 (16)
C6—C5—H5	119.8	C12—N1—Sm1	119.68 (14)
C4—C5—H5	119.8	C10—N2—C11	117.88 (18)
C5—C6—C7	121.1 (2)	C10—N2—Sm1	120.43 (14)
C5—C6—H6	119.4	C11—N2—Sm1	121.67 (14)
C7—C6—H6	119.4	C13—O1—Sm1	93.45 (12)
C8—C7—C11	117.8 (2)	C13—O2—Sm1^{i}	149.14 (14)
C8—C7—C6	122.6 (2)	C13—O2—Sm1	94.89 (12)
C11—C7—C6	119.6 (2)	Sm1^{i}—O2—Sm1	106.72 (5)
C9—C8—C7	119.5 (2)	C16—O3—Sm1	91.82 (14)
C9—C8—H8	120.2	C16—O4—Sm1	93.81 (14)
C7—C8—H8	120.2	C19—O5—Sm1	137.89 (15)
C8—C9—C10	119.1 (2)	C19—O6—Sm1^{i}	137.17 (14)

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

Fig. 1


C14
C15
C13
O1
C9
C8
C10
C7
C6
C11
Sm1i
O2
N2
C4
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C12
Sm1
N1
C3
O6
C19
C1
C2
C21
O3
O4
O5
C18
C16
C20
C17