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# *catena*-Poly[[[aqua[3-(3-hydroxyphenyl)-prop-2-enoato]samarium(III)]-bis[$\mu_2$-3-(3-hydroxyphenyl)prop-2-enoato]] monohydrate]

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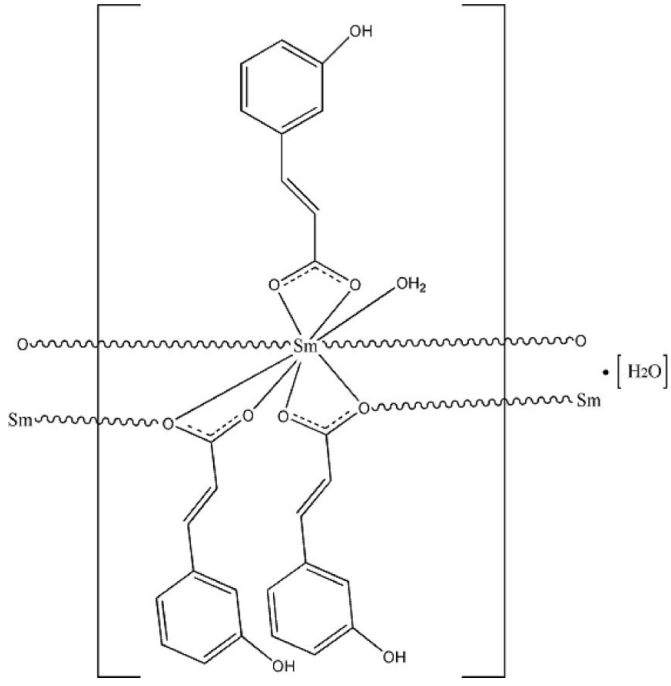
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.014; $wR$ factor = 0.037; data-to-parameter ratio = 12.7.

The title $Sm^{III}$ compound, $\{[Sm(C_9H_7O_3)_3(H_2O)]\cdot H_2O\}_n$, was obtained under hydrothermal conditions. Its structure is isotypic with the analogous Eu complex. The latter was reported incorrectly in space group $P1$ by Yan *et al.* [*J. Mol. Struct.* (2008), **891**, 298–304]. This was corrected by Marsh [*Acta Cryst.* B**65**, 782–783] to $P\overline{1}$. The $Sm^{III}$ ion is nine-coordinated by O atoms from one coordinating water molecule and the remaining ones from the 3-(3-hydroxyphenyl)prop-2-enoatate anions (one bidentate, two bidentate and bridging, two monodentate bridging), leading to a distorted tricapped trigonal–prismatic coordination polyhedron surrounded by solvent water molecules. In the crystal, extensive intermolecular O—H···O hydrogen-bonding interactions and $\pi$–$\pi$ interactions [centroid–centroid separation = 3.9393 (1) Å] lead to the formation of a three-dimensional supramolecular network.

## Related literature

For the isotypic Eu structure, see: Yan *et al.* (2008) and for the corrected space-group assignment, see: Marsh (2009). For related structures, see: Niu *et al.* (2008); Tang *et al.* (2009); Wang & Feng (2010); Xue *et al.* (2007); Ye *et al.* (2005).




## Experimental

### Crystal data

$[Sm(C_9H_7O_3)_3(H_2O)]\cdot H_2O$
$M_r$ = 675.82
Triclinic, $P\overline{1}$
$a$ = 7.9411 (1) Å
$b$ = 13.0312 (2) Å
$c$ = 13.6564 (2) Å
$\alpha$ = 97.356 (1)°
$\beta$ = 97.120 (1)°
$\gamma$ = 103.739 (1)°
$V$ = 1343.87 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 2.25 mm$^{-1}$
$T$ = 296 K
0.52 × 0.24 × 0.15 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.53, $T_{max}$ = 0.71
17958 measured reflections
4722 independent reflections
4590 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.037
$S$ = 1.04
4722 reflections
373 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$WA$···O5$^{i}$ | 0.82 (2) | 2.02 (2) | 2.8183 (18) | 163 (2) |
| O3—H3···O8$^{ii}$ | 0.91 (2) | 1.76 (2) | 2.6692 (19) | 176 (3) |
| O6—H6···O7$^{iii}$ | 0.92 (2) | 1.78 (2) | 2.7005 (19) | 174 (3) |
| O2$W$—H2$WA$···O9$^{iv}$ | 0.84 (2) | 2.15 (2) | 2.947 (4) | 158 (3) |
| O1$W$—H1$WB$···O2$W^{v}$ | 0.83 (2) | 1.86 (2) | 2.688 (2) | 175 (2) |
| O2$W$—H2$WB$···O3$^{vi}$ | 0.81 (2) | 1.98 (2) | 2.790 (3) | 173 (4) |

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

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: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2052).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, m543–m544 [doi:10.1107/S1600536812013724]

## *catena*-Poly[[[aqua[3-(3-hydroxyphenyl)prop-2-enoato]samarium(III)]-bis-[$\mu_2$-3-(3-hydroxyphenyl)prop-2-enoato]] monohydrate]

**Jing-ke Guo and Yi-Hang Wen**

### Comment

It is well known that metal and appropriate ligand are the keys for construction of metal-organic frameworks. Here we choose 3-hydroxycinnamic acid as a ligand due to its unique ability to form stable chelates in diverse coordination modes. Reserches on the compounds containing metal ions and 3-hydroxycinnamic acid have been reported (Niu *et al.* (2008); Xue *et al.*(2007); Ye *et al.*(2005)). Hererin we report a $Sm^{III}$ compound, $Sm(C_9H_7O_3)_3(H_2O).(H_2O)$, derived from 3-hydroxycinnamic acid ($H_2L$),which is not the first rare-earth complex of this ligand. It is isostructural to the Eu complex, Firstly wrongly in P1 by Yan *et al.*, in 2008, this was then corrected by Marsh to P-1 in 2009.

As is shown in Fig. 1, the structrue contains only one nine-coordinated $Sm^{(III)}$ ions which is coordinated by eight oxygen atoms from carboxylate groups in four 3-hydroxyphenyl anions and one oxygen atom from the water molecule, leading to a distored tricapped trigonal prism structure surrounded by solvent $H_2O$ molecule.

In the structure,the 3-hydroxycinnamic acids coordinate *via* three chelating carboxylate groups and two oxygen atoms of another two carboxylate groups bridging two $Sm^{(III)}$ ions [Sm—O distances in the range of 2.3695 (11) and 2.5861 (11) Å], to form a one-dimensional chain with Sm···Sm 4.0887 (1) Å. Furthermore,the oxygen atom in the coordinated water molecule [Sm—O distance 2.4517 (13) Å] completes the nine-coordinated configuration of Sm. In addition,there are one lattice $H_2O$ molecule in the crystal structure. Intermolecular O—H···O and C—H···O hydrogen bonds connect the molecules to form a three-dimensional supramolecular skeleton (Fig. 2).

### Experimental

A mixture of $Sm(NO_3)_3$(0.1682 g, 0.5 mmol),3-hydroxycinnamic acid (0.2462 g, 1.5 mmol) and 4,4-bipyridine (0.2343 g, 1.5 mmol) was dissolved in a 16 mL EtOH/$H_2O$(*v*/*v*,1:15) and then sealed in a 25 ml stainless steel reactor with a telflon liner and heated at 413 K for 72 h, and then cooled to room temperature over 3 days. Then, the reactor was cooled to room temperature at a speed of 5 degrees per hour. Yellow single crystals of title compound were obtained by slow evaporation of the filtrate over a few days.

### Refinement

The carbon-bound H-atoms were positioned geometrically and included in the refinement using a riding model [C—H 0.93 Å $U_{iso}$(H) = 1.2$U_{eq}$(C)]. Water H atoms were located in different maps and refined with distance restraints of O—H = 0.85 (2) Å and H—H = 1.35 Å, with displacement parameters set at 1.5$U_{eq}$(O).

### Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97*

(Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

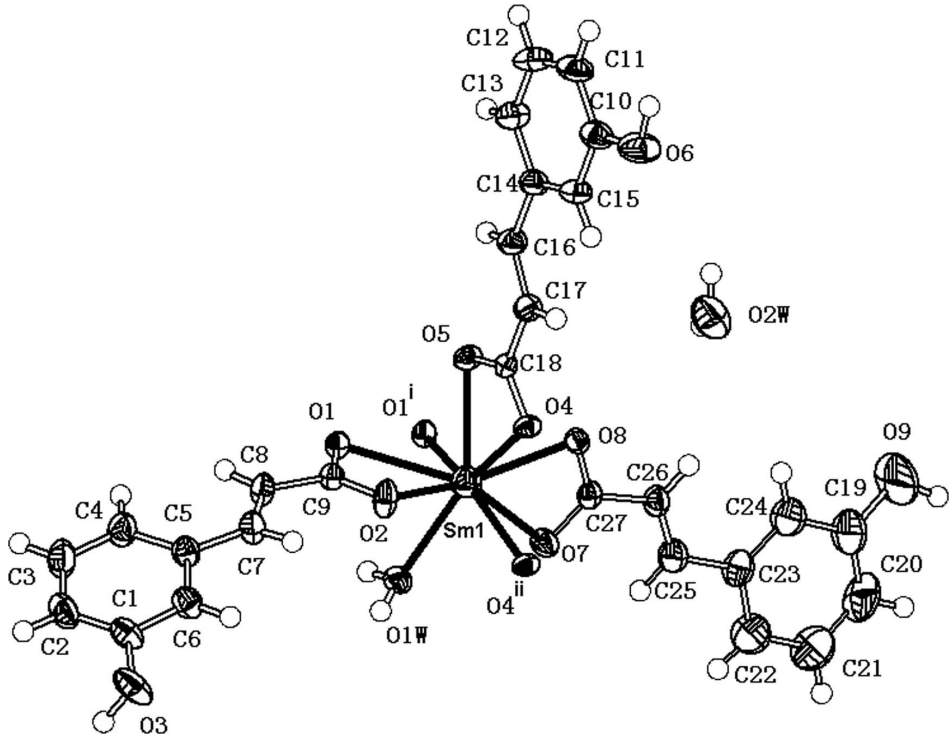


**Figure 1**

The molecular structure of title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) -*x*,-*y* + 1,-*z* + 1; (ii) -*x* + 1,-*y* + 1,-*z* + 1.]

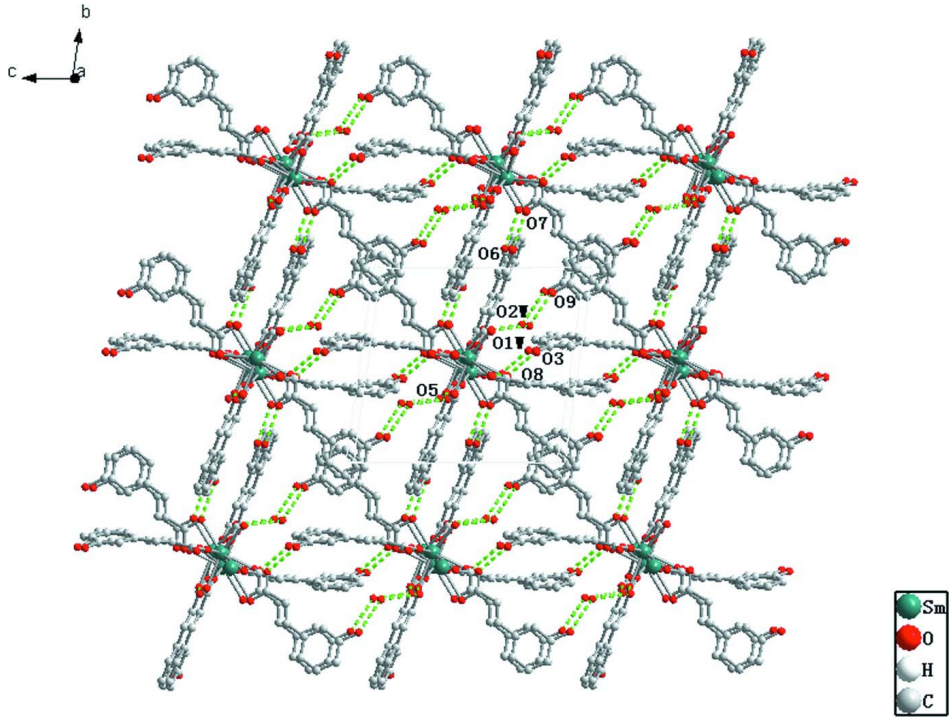


**Figure 2**

View of the supramolecular network conneted by hydrogen bonds.

**_catena_-Poly[[[aqua[3-(3-hydroxyphenyl)prop-2-enoato]samarium(III)]- bis[$\mu_2$-3-(3-hydroxyphenyl)prop-2-enoato]] monohydrate]**

*Crystal data*

$[Sm(C_9H_7O_3)_3(H_2O)]\cdot H_2O$
$M_r = 675.82$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.9411\ (1)$ Å
$b = 13.0312\ (2)$ Å
$c = 13.6564\ (2)$ Å
$\alpha = 97.356\ (1)°$
$\beta = 97.120\ (1)°$
$\gamma = 103.739\ (1)°$
$V = 1343.87\ (3)$ Å$^3$
$Z = 2$
$F(000) = 674$
$D_x = 1.670$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9871 reflections
$\theta = 1.6–25.0°$
$\mu = 2.25$ mm$^{-1}$
$T = 296$ K
Block, yellow
0.52 × 0.24 × 0.15 mm

*Data collection*

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.53$, $T_{max} = 0.71$
17958 measured reflections
4722 independent reflections
4590 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = -9\rightarrow9$
$k = -15\rightarrow15$
$l = -16\rightarrow16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.014$
$wR(F^2) = 0.037$
$S = 1.04$
4722 reflections
373 parameters
10 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
$w = 1/[\sigma^2(F_o^2) + (0.0243P)^2 + 0.3656P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.40$ e Å$^{-3}$
$\Delta\rho_{min} = -0.47$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sm1 | 0.231707 (9) | 0.462033 (5) | 0.480253 (5) | 0.01695 (4) |
| O1 | 0.06012 (15) | 0.55519 (9) | 0.59671 (8) | 0.0240 (2) |
| O1W | 0.07151 (18) | 0.32289 (11) | 0.56401 (11) | 0.0324 (3) |
| H1WA | −0.034 (2) | 0.318 (2) | 0.5643 (17) | 0.049* |
| H1WB | 0.109 (3) | 0.312 (2) | 0.6205 (14) | 0.049* |
| O2 | 0.32583 (16) | 0.54888 (12) | 0.65526 (9) | 0.0349 (3) |
| O2W | 0.7925 (2) | 0.70266 (18) | 0.25319 (14) | 0.0629 (5) |
| H2WA | 0.786 (4) | 0.7600 (17) | 0.232 (3) | 0.094* |
| H2WB | 0.697 (3) | 0.661 (2) | 0.232 (3) | 0.094* |
| O3 | 0.4554 (2) | 0.56809 (15) | 1.19165 (12) | 0.0515 (4) |
| H3 | 0.401 (3) | 0.5246 (19) | 1.2314 (18) | 0.062* |
| O4 | 0.51185 (15) | 0.59885 (9) | 0.47391 (9) | 0.0240 (3) |
| O5 | 0.26831 (15) | 0.64608 (9) | 0.43899 (10) | 0.0278 (3) |
| O6 | 1.0331 (2) | 1.09500 (12) | 0.39523 (14) | 0.0506 (4) |
| H6 | 1.080 (3) | 1.1627 (15) | 0.382 (2) | 0.061* |
| O7 | 0.19076 (17) | 0.29241 (9) | 0.36232 (9) | 0.0306 (3) |
| O8 | 0.28389 (16) | 0.44152 (9) | 0.30584 (9) | 0.0259 (3) |
| O9 | 0.3333 (5) | 0.1288 (2) | −0.16532 (17) | 0.1181 (11) |
| H9 | 0.351 (6) | 0.077 (3) | −0.215 (3) | 0.142* |
| C1 | 0.3318 (3) | 0.59470 (16) | 1.12695 (14) | 0.0358 (4) |
| C2 | 0.1850 (3) | 0.62021 (18) | 1.15591 (15) | 0.0437 (5) |
| H2A | 0.1672 | 0.6218 | 1.2221 | 0.052* |
| C3 | 0.0638 (3) | 0.6435 (2) | 1.08592 (16) | 0.0479 (6) |
| H3A | −0.0346 | 0.6618 | 1.1056 | 0.057* |
| C4 | 0.0877 (3) | 0.63986 (18) | 0.98720 (15) | 0.0401 (5) |

| | | | | |
|---|---|---|---|---|
| H4A | 0.0039 | 0.6541 | 0.9406 | 0.048* |
| C5 | 0.2359 (3) | 0.61510 (15) | 0.95721 (14) | 0.0313 (4) |
| C6 | 0.3595 (3) | 0.59493 (16) | 1.02878 (14) | 0.0349 (4) |
| H6A | 0.4621 | 0.5814 | 1.0104 | 0.042* |
| C7 | 0.2629 (2) | 0.60020 (16) | 0.85277 (14) | 0.0320 (4) |
| H7A | 0.3726 | 0.5922 | 0.8417 | 0.038* |
| C8 | 0.1498 (2) | 0.59684 (16) | 0.77289 (13) | 0.0306 (4) |
| H8A | 0.0447 | 0.6140 | 0.7811 | 0.037* |
| C9 | 0.1830 (2) | 0.56691 (14) | 0.67091 (13) | 0.0237 (4) |
| C10 | 0.8553 (3) | 1.07639 (15) | 0.38269 (15) | 0.0351 (4) |
| C11 | 0.7683 (3) | 1.14997 (15) | 0.35253 (16) | 0.0406 (5) |
| H11A | 0.8315 | 1.2160 | 0.3411 | 0.049* |
| C12 | 0.5879 (3) | 1.12497 (16) | 0.33946 (18) | 0.0457 (5) |
| H12A | 0.5299 | 1.1749 | 0.3196 | 0.055* |
| C13 | 0.4906 (3) | 1.02652 (16) | 0.35534 (17) | 0.0395 (5) |
| H13A | 0.3686 | 1.0104 | 0.3454 | 0.047* |
| C14 | 0.5770 (3) | 0.95222 (14) | 0.38628 (14) | 0.0305 (4) |
| C15 | 0.7603 (3) | 0.97840 (14) | 0.40027 (15) | 0.0329 (4) |
| H15A | 0.8194 | 0.9296 | 0.4216 | 0.040* |
| C16 | 0.4745 (3) | 0.84864 (14) | 0.40343 (14) | 0.0306 (4) |
| H16A | 0.3529 | 0.8359 | 0.3920 | 0.037* |
| C17 | 0.5399 (2) | 0.77163 (14) | 0.43369 (14) | 0.0291 (4) |
| H17A | 0.6614 | 0.7836 | 0.4458 | 0.035* |
| C18 | 0.4330 (2) | 0.66875 (13) | 0.44924 (12) | 0.0214 (3) |
| C19 | 0.2960 (5) | 0.0830 (2) | −0.0827 (2) | 0.0676 (8) |
| C20 | 0.2780 (5) | −0.0240 (2) | −0.0819 (2) | 0.0729 (9) |
| H20A | 0.2905 | −0.0681 | −0.1383 | 0.087* |
| C21 | 0.2415 (5) | −0.0653 (2) | 0.0023 (3) | 0.0786 (10) |
| H21A | 0.2308 | −0.1377 | 0.0036 | 0.094* |
| C22 | 0.2202 (4) | −0.0002 (2) | 0.0858 (2) | 0.0643 (8) |
| H22A | 0.1926 | −0.0294 | 0.1422 | 0.077* |
| C23 | 0.2398 (3) | 0.10820 (18) | 0.08566 (17) | 0.0436 (5) |
| C24 | 0.2779 (4) | 0.1496 (2) | 0.00018 (18) | 0.0572 (7) |
| H24A | 0.2912 | 0.2222 | −0.0014 | 0.069* |
| C25 | 0.2225 (3) | 0.17526 (16) | 0.17687 (15) | 0.0390 (5) |
| H25A | 0.1776 | 0.1391 | 0.2262 | 0.047* |
| C26 | 0.2632 (3) | 0.28090 (15) | 0.19707 (14) | 0.0319 (4) |
| H26A | 0.3052 | 0.3196 | 0.1486 | 0.038* |
| C27 | 0.2452 (2) | 0.34016 (14) | 0.29289 (13) | 0.0241 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sm1 | 0.01437 (6) | 0.01882 (5) | 0.01808 (6) | 0.00429 (3) | 0.00325 (3) | 0.00391 (3) |
| O1 | 0.0194 (6) | 0.0320 (6) | 0.0198 (6) | 0.0078 (5) | 0.0009 (5) | 0.0018 (5) |
| O1W | 0.0274 (7) | 0.0365 (7) | 0.0393 (8) | 0.0103 (6) | 0.0122 (6) | 0.0173 (6) |
| O2 | 0.0209 (6) | 0.0605 (9) | 0.0234 (6) | 0.0171 (6) | 0.0007 (5) | −0.0023 (6) |
| O2W | 0.0519 (11) | 0.0872 (14) | 0.0500 (11) | 0.0134 (10) | 0.0081 (8) | 0.0216 (10) |
| O3 | 0.0422 (9) | 0.0771 (11) | 0.0373 (8) | 0.0086 (8) | 0.0032 (7) | 0.0328 (8) |
| O4 | 0.0185 (6) | 0.0208 (6) | 0.0340 (7) | 0.0063 (5) | 0.0027 (5) | 0.0084 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O5 | 0.0190 (6) | 0.0254 (6) | 0.0420 (7) | 0.0076 (5) | 0.0066 (5) | 0.0109 (5) |
| O6 | 0.0413 (9) | 0.0343 (8) | 0.0739 (12) | −0.0010 (7) | 0.0068 (8) | 0.0225 (8) |
| O7 | 0.0377 (7) | 0.0244 (6) | 0.0275 (7) | 0.0027 (5) | 0.0086 (6) | 0.0033 (5) |
| O8 | 0.0275 (6) | 0.0257 (6) | 0.0250 (6) | 0.0059 (5) | 0.0077 (5) | 0.0046 (5) |
| O9 | 0.224 (3) | 0.0984 (18) | 0.0477 (12) | 0.057 (2) | 0.0579 (17) | 0.0054 (12) |
| C1 | 0.0355 (11) | 0.0413 (11) | 0.0270 (10) | 0.0019 (8) | 0.0010 (8) | 0.0113 (8) |
| C2 | 0.0549 (14) | 0.0517 (13) | 0.0255 (10) | 0.0117 (10) | 0.0127 (10) | 0.0080 (9) |
| C3 | 0.0507 (14) | 0.0636 (15) | 0.0366 (12) | 0.0248 (11) | 0.0167 (10) | 0.0062 (10) |
| C4 | 0.0420 (12) | 0.0539 (12) | 0.0298 (10) | 0.0225 (10) | 0.0066 (9) | 0.0067 (9) |
| C5 | 0.0336 (10) | 0.0350 (10) | 0.0244 (9) | 0.0083 (8) | 0.0038 (8) | 0.0033 (7) |
| C6 | 0.0297 (10) | 0.0445 (11) | 0.0302 (10) | 0.0073 (8) | 0.0038 (8) | 0.0095 (8) |
| C7 | 0.0271 (9) | 0.0444 (11) | 0.0255 (9) | 0.0113 (8) | 0.0050 (8) | 0.0039 (8) |
| C8 | 0.0260 (9) | 0.0455 (11) | 0.0231 (9) | 0.0159 (8) | 0.0047 (8) | 0.0022 (8) |
| C9 | 0.0225 (9) | 0.0256 (8) | 0.0217 (9) | 0.0056 (7) | 0.0024 (7) | 0.0017 (7) |
| C10 | 0.0425 (12) | 0.0257 (9) | 0.0333 (10) | 0.0021 (8) | 0.0039 (9) | 0.0059 (8) |
| C11 | 0.0544 (13) | 0.0226 (9) | 0.0425 (12) | 0.0029 (9) | 0.0067 (10) | 0.0115 (8) |
| C12 | 0.0588 (15) | 0.0289 (10) | 0.0549 (14) | 0.0175 (10) | 0.0061 (11) | 0.0179 (10) |
| C13 | 0.0418 (12) | 0.0326 (10) | 0.0466 (12) | 0.0125 (9) | 0.0050 (10) | 0.0121 (9) |
| C14 | 0.0398 (11) | 0.0236 (9) | 0.0287 (9) | 0.0075 (8) | 0.0070 (8) | 0.0061 (7) |
| C15 | 0.0391 (11) | 0.0235 (9) | 0.0373 (10) | 0.0069 (8) | 0.0053 (9) | 0.0116 (8) |
| C16 | 0.0304 (10) | 0.0258 (9) | 0.0370 (10) | 0.0069 (7) | 0.0072 (8) | 0.0089 (8) |
| C17 | 0.0239 (9) | 0.0256 (9) | 0.0389 (10) | 0.0052 (7) | 0.0087 (8) | 0.0086 (8) |
| C18 | 0.0215 (9) | 0.0216 (8) | 0.0222 (8) | 0.0068 (6) | 0.0047 (7) | 0.0036 (6) |
| C19 | 0.096 (2) | 0.0696 (18) | 0.0382 (14) | 0.0266 (16) | 0.0186 (14) | −0.0042 (12) |
| C20 | 0.095 (2) | 0.0618 (18) | 0.0569 (18) | 0.0250 (16) | 0.0176 (16) | −0.0221 (14) |
| C21 | 0.116 (3) | 0.0413 (14) | 0.074 (2) | 0.0186 (15) | 0.0223 (19) | −0.0111 (14) |
| C22 | 0.091 (2) | 0.0405 (13) | 0.0580 (16) | 0.0123 (13) | 0.0192 (15) | −0.0024 (12) |
| C23 | 0.0502 (13) | 0.0402 (12) | 0.0371 (12) | 0.0117 (10) | 0.0068 (10) | −0.0057 (9) |
| C24 | 0.086 (2) | 0.0462 (13) | 0.0402 (13) | 0.0215 (13) | 0.0153 (13) | −0.0018 (10) |
| C25 | 0.0472 (12) | 0.0391 (11) | 0.0306 (10) | 0.0121 (9) | 0.0084 (9) | 0.0021 (8) |
| C26 | 0.0350 (10) | 0.0364 (10) | 0.0251 (9) | 0.0112 (8) | 0.0072 (8) | 0.0019 (8) |
| C27 | 0.0175 (8) | 0.0307 (9) | 0.0240 (9) | 0.0070 (7) | 0.0024 (7) | 0.0030 (7) |

*Geometric parameters (Å, º)*

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| Sm1—O1$^{i}$ | 2.3695 (11) | C5—C6 | 1.392 (3) |
| Sm1—O4$^{ii}$ | 2.3973 (11) | C5—C7 | 1.464 (3) |
| Sm1—O1W | 2.4517 (13) | C6—H6A | 0.9300 |
| Sm1—O2 | 2.4524 (12) | C7—C8 | 1.313 (3) |
| Sm1—O8 | 2.4598 (12) | C7—H7A | 0.9300 |
| Sm1—O7 | 2.4905 (12) | C8—C9 | 1.470 (2) |
| Sm1—O5 | 2.4919 (12) | C8—H8A | 0.9300 |
| Sm1—O4 | 2.5176 (11) | C10—C11 | 1.382 (3) |
| Sm1—O1 | 2.5861 (11) | C10—C15 | 1.387 (3) |
| Sm1—C27 | 2.8616 (17) | C11—C12 | 1.375 (3) |
| Sm1—C9 | 2.8959 (17) | C11—H11A | 0.9300 |
| Sm1—C18 | 2.8991 (16) | C12—C13 | 1.390 (3) |
| O1—C9 | 1.283 (2) | C12—H12A | 0.9300 |
| O1—Sm1$^{i}$ | 2.3695 (11) | C13—C14 | 1.391 (3) |
| O1W—H1WA | 0.824 (15) | C13—H13A | 0.9300 |

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| O1W—H1WB | 0.834 (16) | C14—C15 | 1.397 (3) |
| O2—C9 | 1.249 (2) | C14—C16 | 1.465 (2) |
| O2W—H2WA | 0.844 (17) | C15—H15A | 0.9300 |
| O2W—H2WB | 0.814 (17) | C16—C17 | 1.322 (3) |
| O3—C1 | 1.374 (3) | C16—H16A | 0.9300 |
| O3—H3 | 0.906 (17) | C17—C18 | 1.463 (2) |
| O4—C18 | 1.278 (2) | C17—H17A | 0.9300 |
| O4—Sm1$^{ii}$ | 2.3973 (11) | C19—C20 | 1.369 (4) |
| O5—C18 | 1.256 (2) | C19—C24 | 1.379 (3) |
| O6—C10 | 1.360 (3) | C20—C21 | 1.365 (5) |
| O6—H6 | 0.923 (17) | C20—H20A | 0.9300 |
| O7—C27 | 1.264 (2) | C21—C22 | 1.384 (4) |
| O8—C27 | 1.267 (2) | C21—H21A | 0.9300 |
| O9—C19 | 1.374 (4) | C22—C23 | 1.384 (3) |
| O9—H9 | 0.944 (19) | C22—H22A | 0.9300 |
| C1—C2 | 1.375 (3) | C23—C24 | 1.384 (4) |
| C1—C6 | 1.385 (3) | C23—C25 | 1.468 (3) |
| C2—C3 | 1.385 (3) | C24—H24A | 0.9300 |
| C2—H2A | 0.9300 | C25—C26 | 1.321 (3) |
| C3—C4 | 1.381 (3) | C25—H25A | 0.9300 |
| C3—H3A | 0.9300 | C26—C27 | 1.473 (2) |
| C4—C5 | 1.387 (3) | C26—H26A | 0.9300 |
| C4—H4A | 0.9300 | | |

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| O1$^{i}$—Sm1—O4$^{ii}$ | 155.55 (4) | C1—C2—H2A | 120.2 |
| O1$^{i}$—Sm1—O1W | 79.70 (5) | C3—C2—H2A | 120.2 |
| O4$^{ii}$—Sm1—O1W | 87.34 (4) | C4—C3—C2 | 120.7 (2) |
| O1$^{i}$—Sm1—O2 | 119.15 (4) | C4—C3—H3A | 119.7 |
| O4$^{ii}$—Sm1—O2 | 78.18 (4) | C2—C3—H3A | 119.7 |
| O1W—Sm1—O2 | 79.90 (5) | C3—C4—C5 | 120.3 (2) |
| O1$^{i}$—Sm1—O8 | 82.67 (4) | C3—C4—H4A | 119.9 |
| O4$^{ii}$—Sm1—O8 | 88.82 (4) | C5—C4—H4A | 119.9 |
| O1W—Sm1—O8 | 126.86 (4) | C4—C5—C6 | 118.54 (18) |
| O2—Sm1—O8 | 150.00 (4) | C4—C5—C7 | 123.46 (18) |
| O1$^{i}$—Sm1—O7 | 81.62 (4) | C6—C5—C7 | 117.80 (17) |
| O4$^{ii}$—Sm1—O7 | 75.09 (4) | C1—C6—C5 | 120.92 (19) |
| O1W—Sm1—O7 | 75.65 (4) | C1—C6—H6A | 119.5 |
| O2—Sm1—O7 | 144.28 (5) | C5—C6—H6A | 119.5 |
| O8—Sm1—O7 | 52.30 (4) | C8—C7—C5 | 127.42 (18) |
| O1$^{i}$—Sm1—O5 | 81.25 (4) | C8—C7—H7A | 116.3 |
| O4$^{ii}$—Sm1—O5 | 119.02 (4) | C5—C7—H7A | 116.3 |
| O1W—Sm1—O5 | 147.03 (4) | C7—C8—C9 | 122.50 (17) |
| O2—Sm1—O5 | 86.30 (5) | C7—C8—H8A | 118.8 |
| O8—Sm1—O5 | 76.50 (4) | C9—C8—H8A | 118.8 |
| O7—Sm1—O5 | 127.52 (4) | O2—C9—O1 | 119.34 (15) |
| O1$^{i}$—Sm1—O4 | 130.35 (4) | O2—C9—C8 | 121.45 (16) |
| O4$^{ii}$—Sm1—O4 | 67.43 (4) | O1—C9—C8 | 119.16 (15) |
| O1W—Sm1—O4 | 148.72 (4) | O2—C9—Sm1 | 57.08 (9) |
| O2—Sm1—O4 | 77.13 (4) | O1—C9—Sm1 | 63.25 (8) |

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| O8—Sm1—O4 | 72.92 (4) | C8—C9—Sm1 | 167.72 (13) |
| O7—Sm1—O4 | 112.86 (4) | O6—C10—C11 | 122.73 (17) |
| O5—Sm1—O4 | 51.62 (4) | O6—C10—C15 | 117.38 (19) |
| O1$^{i}$—Sm1—O1 | 67.98 (4) | C11—C10—C15 | 119.9 (2) |
| O4$^{ii}$—Sm1—O1 | 128.01 (4) | C12—C11—C10 | 119.62 (18) |
| O1W—Sm1—O1 | 73.82 (4) | C12—C11—H11A | 120.2 |
| O2—Sm1—O1 | 51.34 (4) | C10—C11—H11A | 120.2 |
| O8—Sm1—O1 | 140.98 (4) | C11—C12—C13 | 121.2 (2) |
| O7—Sm1—O1 | 139.96 (4) | C11—C12—H12A | 119.4 |
| O5—Sm1—O1 | 74.17 (4) | C13—C12—H12A | 119.4 |
| O4—Sm1—O1 | 106.71 (4) | C12—C13—C14 | 119.5 (2) |
| O1$^{i}$—Sm1—C27 | 82.20 (4) | C12—C13—H13A | 120.2 |
| O4$^{ii}$—Sm1—C27 | 80.18 (5) | C14—C13—H13A | 120.2 |
| O1W—Sm1—C27 | 101.49 (5) | C13—C14—C15 | 118.97 (18) |
| O2—Sm1—C27 | 158.23 (5) | C13—C14—C16 | 119.57 (18) |
| O8—Sm1—C27 | 26.17 (5) | C15—C14—C16 | 121.46 (17) |
| O7—Sm1—C27 | 26.16 (5) | C10—C15—C14 | 120.72 (19) |
| O5—Sm1—C27 | 102.28 (5) | C10—C15—H15A | 119.6 |
| O4—Sm1—C27 | 92.42 (4) | C14—C15—H15A | 119.6 |
| O1—Sm1—C27 | 150.18 (4) | C17—C16—C14 | 125.68 (18) |
| O1$^{i}$—Sm1—C9 | 93.84 (4) | C17—C16—H16A | 117.2 |
| O4$^{ii}$—Sm1—C9 | 102.04 (5) | C14—C16—H16A | 117.2 |
| O1W—Sm1—C9 | 72.73 (5) | C16—C17—C18 | 124.04 (17) |
| O2—Sm1—C9 | 25.32 (5) | C16—C17—H17A | 118.0 |
| O8—Sm1—C9 | 158.51 (5) | C18—C17—H17A | 118.0 |
| O7—Sm1—C9 | 148.35 (4) | O5—C18—O4 | 118.84 (15) |
| O5—Sm1—C9 | 82.02 (5) | O5—C18—C17 | 123.16 (16) |
| O4—Sm1—C9 | 94.00 (4) | O4—C18—C17 | 118.00 (15) |
| O1—Sm1—C9 | 26.30 (4) | O5—C18—Sm1 | 58.79 (8) |
| C27—Sm1—C9 | 173.57 (5) | O4—C18—Sm1 | 60.05 (8) |
| O1$^{i}$—Sm1—C18 | 105.70 (4) | C17—C18—Sm1 | 178.01 (12) |
| O4$^{ii}$—Sm1—C18 | 93.51 (4) | C20—C19—O9 | 121.7 (2) |
| O1W—Sm1—C18 | 160.17 (5) | C20—C19—C24 | 121.1 (3) |
| O2—Sm1—C18 | 80.89 (5) | O9—C19—C24 | 117.2 (3) |
| O8—Sm1—C18 | 72.97 (4) | C21—C20—C19 | 119.3 (2) |
| O7—Sm1—C18 | 123.71 (4) | C21—C20—H20A | 120.3 |
| O5—Sm1—C18 | 25.53 (4) | C19—C20—H20A | 120.3 |
| O4—Sm1—C18 | 26.09 (4) | C20—C21—C22 | 120.5 (3) |
| O1—Sm1—C18 | 90.30 (4) | C20—C21—H21A | 119.7 |
| C27—Sm1—C18 | 98.18 (5) | C22—C21—H21A | 119.7 |
| C9—Sm1—C18 | 87.75 (5) | C23—C22—C21 | 120.3 (3) |
| C9—O1—Sm1$^{i}$ | 155.04 (11) | C23—C22—H22A | 119.9 |
| C9—O1—Sm1 | 90.44 (9) | C21—C22—H22A | 119.9 |
| Sm1$^{i}$—O1—Sm1 | 112.02 (4) | C22—C23—C24 | 118.8 (2) |
| Sm1—O1W—H1WA | 117.4 (17) | C22—C23—C25 | 118.7 (2) |
| Sm1—O1W—H1WB | 123.4 (17) | C24—C23—C25 | 122.5 (2) |
| H1WA—O1W—H1WB | 104.8 (19) | C19—C24—C23 | 119.9 (3) |
| C9—O2—Sm1 | 97.61 (10) | C19—C24—H24A | 120.0 |
| H2WA—O2W—H2WB | 105 (2) | C23—C24—H24A | 120.0 |

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| C1—O3—H3 | 109.8 (18) | C26—C25—C23 | 127.6 (2) |
| C18—O4—Sm1$^{ii}$ | 153.49 (10) | C26—C25—H25A | 116.2 |
| C18—O4—Sm1 | 93.86 (9) | C23—C25—H25A | 116.2 |
| Sm1$^{ii}$—O4—Sm1 | 112.57 (4) | C25—C26—C27 | 123.00 (19) |
| C18—O5—Sm1 | 95.67 (10) | C25—C26—H26A | 118.5 |
| C10—O6—H6 | 108.7 (17) | C27—C26—H26A | 118.5 |
| C27—O7—Sm1 | 93.54 (10) | O7—C27—O8 | 119.10 (15) |
| C27—O8—Sm1 | 94.92 (10) | O7—C27—C26 | 121.68 (16) |
| C19—O9—H9 | 109 (3) | O8—C27—C26 | 119.22 (16) |
| O3—C1—C2 | 122.80 (18) | O7—C27—Sm1 | 60.30 (9) |
| O3—C1—C6 | 117.30 (19) | O8—C27—Sm1 | 58.92 (8) |
| C2—C1—C6 | 119.90 (19) | C26—C27—Sm1 | 176.60 (13) |
| C1—C2—C3 | 119.56 (19) | | |

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| O1$^{i}$—Sm1—O1—C9 | 168.85 (12) | O1$^{i}$—Sm1—C9—O2 | −178.87 (11) |
| O4$^{ii}$—Sm1—O1—C9 | 10.38 (11) | O4$^{ii}$—Sm1—C9—O2 | 19.83 (12) |
| O1W—Sm1—O1—C9 | 83.64 (10) | O1W—Sm1—C9—O2 | 103.17 (12) |
| O2—Sm1—O1—C9 | −6.26 (10) | O8—Sm1—C9—O2 | −99.16 (16) |
| O8—Sm1—O1—C9 | −147.01 (10) | O7—Sm1—C9—O2 | 100.89 (13) |
| O7—Sm1—O1—C9 | 125.36 (10) | O5—Sm1—C9—O2 | −98.27 (11) |
| O5—Sm1—O1—C9 | −104.36 (10) | O4—Sm1—C9—O2 | −47.93 (12) |
| O4—Sm1—O1—C9 | −63.72 (10) | O1—Sm1—C9—O2 | −168.52 (18) |
| C27—Sm1—O1—C9 | 168.52 (10) | C18—Sm1—C9—O2 | −73.28 (12) |
| C18—Sm1—O1—C9 | −84.31 (10) | O1$^{i}$—Sm1—C9—O1 | −10.35 (11) |
| O1$^{i}$—Sm1—O1—Sm1$^{i}$ | 0.0 | O4$^{ii}$—Sm1—C9—O1 | −171.66 (9) |
| O4$^{ii}$—Sm1—O1—Sm1$^{i}$ | −158.47 (4) | O1W—Sm1—C9—O1 | −88.32 (10) |
| O1W—Sm1—O1—Sm1$^{i}$ | −85.21 (6) | O2—Sm1—C9—O1 | 168.52 (17) |
| O2—Sm1—O1—Sm1$^{i}$ | −175.11 (8) | O8—Sm1—C9—O1 | 69.36 (16) |
| O8—Sm1—O1—Sm1$^{i}$ | 44.14 (8) | O7—Sm1—C9—O1 | −90.60 (13) |
| O7—Sm1—O1—Sm1$^{i}$ | −43.49 (8) | O5—Sm1—C9—O1 | 70.24 (9) |
| O5—Sm1—O1—Sm1$^{i}$ | 86.80 (5) | O4—Sm1—C9—O1 | 120.58 (9) |
| O4—Sm1—O1—Sm1$^{i}$ | 127.43 (5) | C18—Sm1—C9—O1 | 95.23 (10) |
| C27—Sm1—O1—Sm1$^{i}$ | −0.32 (11) | O1$^{i}$—Sm1—C9—C8 | 94.1 (6) |
| C9—Sm1—O1—Sm1$^{i}$ | −168.85 (12) | O4$^{ii}$—Sm1—C9—C8 | −67.2 (6) |
| C18—Sm1—O1—Sm1$^{i}$ | 106.84 (5) | O1W—Sm1—C9—C8 | 16.2 (6) |
| O1$^{i}$—Sm1—O2—C9 | 1.29 (13) | O2—Sm1—C9—C8 | −87.0 (6) |
| O4$^{ii}$—Sm1—O2—C9 | −160.19 (12) | O8—Sm1—C9—C8 | 173.9 (5) |
| O1W—Sm1—O2—C9 | −70.81 (11) | O7—Sm1—C9—C8 | 13.9 (6) |
| O8—Sm1—O2—C9 | 133.68 (11) | O5—Sm1—C9—C8 | 174.7 (6) |
| O7—Sm1—O2—C9 | −118.04 (12) | O4—Sm1—C9—C8 | −134.9 (6) |
| O5—Sm1—O2—C9 | 79.13 (11) | O1—Sm1—C9—C8 | 104.5 (6) |
| O4—Sm1—O2—C9 | 130.57 (12) | C18—Sm1—C9—C8 | −160.3 (6) |
| O1—Sm1—O2—C9 | 6.49 (10) | O6—C10—C11—C12 | 178.7 (2) |
| C27—Sm1—O2—C9 | −166.51 (12) | C15—C10—C11—C12 | −0.5 (3) |
| C18—Sm1—O2—C9 | 104.25 (12) | C10—C11—C12—C13 | −0.5 (3) |
| O1$^{i}$—Sm1—O4—C18 | 21.91 (11) | C11—C12—C13—C14 | 0.8 (3) |
| O4$^{ii}$—Sm1—O4—C18 | −177.95 (12) | C12—C13—C14—C15 | −0.3 (3) |
| O1W—Sm1—O4—C18 | −139.30 (10) | C12—C13—C14—C16 | 179.75 (19) |
| O2—Sm1—O4—C18 | −95.58 (10) | O6—C10—C15—C14 | −178.21 (18) |

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| O8—Sm1—O4—C18 | 86.05 (10) | C11—C10—C15—C14 | 1.1 (3) |
| O7—Sm1—O4—C18 | 120.58 (9) | C13—C14—C15—C10 | −0.7 (3) |
| O5—Sm1—O4—C18 | −0.04 (9) | C16—C14—C15—C10 | 179.31 (18) |
| O1—Sm1—O4—C18 | −53.10 (10) | C13—C14—C16—C17 | −179.3 (2) |
| C27—Sm1—O4—C18 | 103.73 (10) | C15—C14—C16—C17 | 0.7 (3) |
| C9—Sm1—O4—C18 | −76.57 (10) | C14—C16—C17—C18 | −179.51 (17) |
| O1$^{i}$—Sm1—O4—Sm1$^{ii}$ | −160.13 (4) | Sm1—O5—C18—O4 | −0.08 (16) |
| O4$^{ii}$—Sm1—O4—Sm1$^{ii}$ | 0.0 | Sm1—O5—C18—C17 | 179.55 (15) |
| O1W—Sm1—O4—Sm1$^{ii}$ | 38.66 (10) | Sm1$^{ii}$—O4—C18—O5 | −175.69 (16) |
| O2—Sm1—O4—Sm1$^{ii}$ | 82.38 (5) | Sm1—O4—C18—O5 | 0.08 (16) |
| O8—Sm1—O4—Sm1$^{ii}$ | −96.00 (5) | Sm1$^{ii}$—O4—C18—C17 | 4.7 (3) |
| O7—Sm1—O4—Sm1$^{ii}$ | −61.47 (6) | Sm1—O4—C18—C17 | −179.57 (13) |
| O5—Sm1—O4—Sm1$^{ii}$ | 177.91 (7) | Sm1$^{ii}$—O4—C18—Sm1 | −175.8 (3) |
| O1—Sm1—O4—Sm1$^{ii}$ | 124.86 (5) | C16—C17—C18—O5 | −3.0 (3) |
| C27—Sm1—O4—Sm1$^{ii}$ | −78.32 (6) | C16—C17—C18—O4 | 176.63 (17) |
| C9—Sm1—O4—Sm1$^{ii}$ | 101.38 (6) | O1$^{i}$—Sm1—C18—O5 | 17.26 (11) |
| C18—Sm1—O4—Sm1$^{ii}$ | 177.95 (12) | O4$^{ii}$—Sm1—C18—O5 | −178.03 (10) |
| O1$^{i}$—Sm1—O5—C18 | −163.20 (10) | O1W—Sm1—C18—O5 | −86.14 (17) |
| O4$^{ii}$—Sm1—O5—C18 | 2.25 (11) | O2—Sm1—C18—O5 | −100.60 (10) |
| O1W—Sm1—O5—C18 | 141.53 (11) | O8—Sm1—C18—O5 | 94.28 (10) |
| O2—Sm1—O5—C18 | 76.54 (10) | O7—Sm1—C18—O5 | 107.58 (10) |
| O8—Sm1—O5—C18 | −78.70 (10) | O4—Sm1—C18—O5 | −179.92 (16) |
| O7—Sm1—O5—C18 | −90.91 (11) | O1—Sm1—C18—O5 | −49.91 (10) |
| O4—Sm1—O5—C18 | 0.04 (9) | C27—Sm1—C18—O5 | 101.40 (10) |
| O1—Sm1—O5—C18 | 127.32 (10) | C9—Sm1—C18—O5 | −76.10 (10) |
| C27—Sm1—O5—C18 | −83.23 (10) | O1$^{i}$—Sm1—C18—O4 | −162.82 (9) |
| C9—Sm1—O5—C18 | 101.64 (10) | O4$^{ii}$—Sm1—C18—O4 | 1.89 (11) |
| O1$^{i}$—Sm1—O7—C27 | 89.35 (11) | O1W—Sm1—C18—O4 | 93.79 (16) |
| O4$^{ii}$—Sm1—O7—C27 | −98.15 (11) | O2—Sm1—C18—O4 | 79.32 (9) |
| O1W—Sm1—O7—C27 | 170.79 (11) | O8—Sm1—C18—O4 | −85.80 (9) |
| O2—Sm1—O7—C27 | −140.97 (10) | O7—Sm1—C18—O4 | −72.50 (10) |
| O8—Sm1—O7—C27 | 2.16 (9) | O5—Sm1—C18—O4 | 179.92 (16) |
| O5—Sm1—O7—C27 | 17.23 (12) | O1—Sm1—C18—O4 | 130.01 (9) |
| O4—Sm1—O7—C27 | −41.05 (11) | C27—Sm1—C18—O4 | −78.68 (10) |
| O1—Sm1—O7—C27 | 129.50 (10) | C9—Sm1—C18—O4 | 103.82 (10) |
| C9—Sm1—O7—C27 | 173.03 (10) | C24—C19—C20—C21 | 0.0 (6) |
| C18—Sm1—O7—C27 | −13.98 (12) | C19—C20—C21—C22 | 0.9 (6) |
| O1$^{i}$—Sm1—O8—C27 | −87.21 (10) | C20—C21—C22—C23 | −1.5 (6) |
| O4$^{ii}$—Sm1—O8—C27 | 69.81 (10) | C21—C22—C23—C24 | 1.1 (5) |
| O1W—Sm1—O8—C27 | −15.98 (12) | C21—C22—C23—C25 | −177.8 (3) |
| O2—Sm1—O8—C27 | 133.36 (11) | C20—C19—C24—C23 | −0.4 (5) |
| O7—Sm1—O8—C27 | −2.16 (9) | O9—C19—C24—C23 | 179.8 (3) |
| O5—Sm1—O8—C27 | −169.92 (10) | C22—C23—C24—C19 | −0.2 (5) |
| O4—Sm1—O8—C27 | 136.53 (10) | C25—C23—C24—C19 | 178.7 (3) |
| O1—Sm1—O8—C27 | −127.82 (10) | C22—C23—C25—C26 | 168.4 (3) |
| C9—Sm1—O8—C27 | −169.02 (11) | C24—C23—C25—C26 | −10.5 (4) |
| C18—Sm1—O8—C27 | 163.84 (11) | C23—C25—C26—C27 | −178.1 (2) |
| O3—C1—C2—C3 | −178.3 (2) | Sm1—O7—C27—O8 | −3.80 (17) |
| C6—C1—C2—C3 | 1.5 (3) | Sm1—O7—C27—C26 | 176.78 (15) |

| | | | |
|---|---|---|---|
| C1—C2—C3—C4 | 0.9 (4) | Sm1—O8—C27—O7 | 3.86 (17) |
| C2—C3—C4—C5 | −1.5 (4) | Sm1—O8—C27—C26 | −176.71 (14) |
| C3—C4—C5—C6 | −0.4 (3) | C25—C26—C27—O7 | 0.8 (3) |
| C3—C4—C5—C7 | 174.3 (2) | C25—C26—C27—O8 | −178.66 (19) |
| O3—C1—C6—C5 | 176.38 (18) | O1$^{i}$—Sm1—C27—O7 | −86.87 (10) |
| C2—C1—C6—C5 | −3.5 (3) | O4$^{ii}$—Sm1—C27—O7 | 76.12 (10) |
| C4—C5—C6—C1 | 2.9 (3) | O1W—Sm1—C27—O7 | −9.11 (11) |
| C7—C5—C6—C1 | −172.11 (18) | O2—Sm1—C27—O7 | 82.40 (16) |
| C4—C5—C7—C8 | −7.3 (3) | O8—Sm1—C27—O7 | −176.12 (17) |
| C6—C5—C7—C8 | 167.4 (2) | O5—Sm1—C27—O7 | −166.09 (10) |
| C5—C7—C8—C9 | −171.47 (18) | O4—Sm1—C27—O7 | 142.72 (10) |
| Sm1—O2—C9—O1 | −11.77 (18) | O1—Sm1—C27—O7 | −86.56 (14) |
| Sm1—O2—C9—C8 | 165.59 (15) | C18—Sm1—C27—O7 | 168.29 (10) |
| Sm1$^{i}$—O1—C9—O2 | 165.90 (18) | O1$^{i}$—Sm1—C27—O8 | 89.25 (10) |
| Sm1—O1—C9—O2 | 11.05 (17) | O4$^{ii}$—Sm1—C27—O8 | −107.76 (10) |
| Sm1$^{i}$—O1—C9—C8 | −11.5 (4) | O1W—Sm1—C27—O8 | 167.01 (10) |
| Sm1—O1—C9—C8 | −166.37 (15) | O2—Sm1—C27—O8 | −101.48 (16) |
| Sm1$^{i}$—O1—C9—Sm1 | 154.8 (3) | O7—Sm1—C27—O8 | 176.12 (17) |
| C7—C8—C9—O2 | −4.1 (3) | O5—Sm1—C27—O8 | 10.03 (10) |
| C7—C8—C9—O1 | 173.30 (18) | O4—Sm1—C27—O8 | −41.16 (10) |
| C7—C8—C9—Sm1 | 75.2 (6) | O1—Sm1—C27—O8 | 89.55 (12) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*WA*···O5$^{i}$ | 0.82 (2) | 2.02 (2) | 2.8183 (18) | 163 (2) |
| O3—H3···O8$^{iii}$ | 0.91 (2) | 1.76 (2) | 2.6692 (19) | 176 (3) |
| O6—H6···O7$^{iv}$ | 0.92 (2) | 1.78 (2) | 2.7005 (19) | 174 (3) |
| O2*W*—H2*WA*···O9$^{v}$ | 0.84 (2) | 2.15 (2) | 2.947 (4) | 158 (3) |
| O1*W*—H1*WB*···O2*W*$^{vi}$ | 0.83 (2) | 1.86 (2) | 2.688 (2) | 175 (2) |
| O2*W*—H2*WB*···O3$^{vi}$ | 0.81 (2) | 1.98 (2) | 2.790 (3) | 173 (4) |

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