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# Crystal structure and Hirshfeld surface analysis of ((*S*,*S*)-2,2′-{(1,2-diphenylethane-1,2-diyl)bis[(azaniumylylidene)methanylylidene]}bis(6-methoxyphenolato))trinitratosamarium(III)

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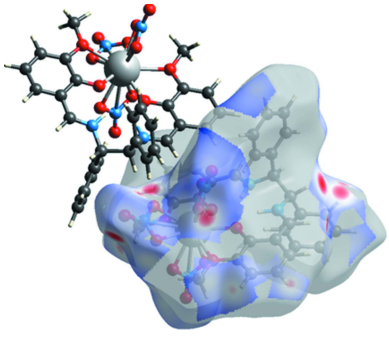
In the title complex, $[Sm(NO_3)_3(C_{30}H_{28}N_2O_4)]$, the Sm atom is surrounded by ten O atoms. The (*S*,*S*)-2,2′-{[(1,2-diphenylethane-1,2-diyl)bis[(azaniumylylidene)methanylylidene]}bis(6-methoxyphenolate) ligand, obtained from *o*-vanillin and (1*S*,2*S*)-(−)-1,2-diphenylethylenediamine, exhibits a slightly distorted planar arrangement of the four coordinated O atoms. In the crystal, the complex shows intramolecular N—H···O hydrogen bonds and weak intermolecular C—H···O hydrogen bonds. The Hirshfeld surface analysis indicates that the most important contributions to the packing are from H···H (33.5%), O···H (34.1%) and C···H (21.7%) contacts.

## 1. Chemical context

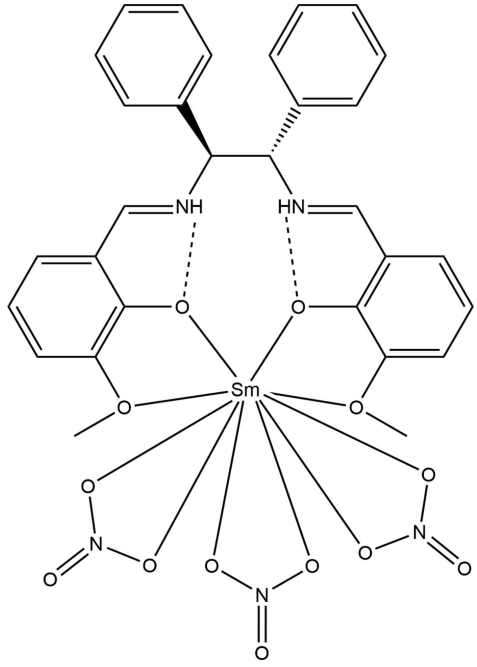
Lanthanide metal complexes can have attractive functions such as magnetism and fluorescence when synthesized with properly designed ligands (Yao *et al.*, 2019; Lin *et al.*, 2009). In recent years, lanthanide complexes that act as single-molecule magnets (SMM) have received much attention (Then *et al.*, 2015). In these complexes, distortion of the coordination geometry is an important factor for magnetic anisotropy and for the resulting SMM properties. However, the coordination chemistry of lanthanides is complicated, and it is necessary to prepare complexes with coordination environments suitable for the required properties. On the other hand, salen ligands are known to form stable chelate complexes with many metals (Cozzi *et al.*, 2004). By incorporating a substituent group into salen ligands, it is possible to easily add more coordination sites and optical functionality such as the antenna effect that depend on intermolecular interactions and arrangements. Hence, functional lanthanide salen complexes have attracted attention (Ren *et al.*, 2016). Accurate data such as bond angles and the geometry of coordination sites obtained based on crystal structure analysis and Hirshfeld surface analysis will be useful for the molecular design of new lanthanide and salen complexes. In this study, we prepared a new $Sm^{III}$–salen complex and report herein on its crystal structure and Hirshfeld surface analysis.



## 2. Structural commentary

The title $Sm^{III}$ complex crystallizes in the monoclinic space group *C*2. The asymmetric unit contains two crystallographically independent molecules. This distorted prismatic

[$SmO_{10}$] complex consists of three bidentate nitrate ions and two pairs of phenolate and methoxy groups of the salen ligand, which is slightly distorted from planar.




The bond distances between the metal center and ligating atoms range from 2.333 (5) to 2.373 (4) Å for the phenolato oxygen atoms, and from 2.606 (5) to 2.621 (6) Å for methoxy oxygen atoms. The bond lengths between the metal center and the nitrate oxygen atoms range from 2.475 (5) to 2.633 (5) Å, showing more flexibility than those of the Schiff base ligand. In the Schiff base ligand, the imine moieties are protonated to form iminium cations, but the C═N bond lengths remain close to those of normal imine bonds at 1.287 (8) and 1.30 (1) Å.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C98—H98$A$···O9$^{i}$ | 0.98 | 2.58 | 3.419 (9) | 144 |
| C91—H91···O27$^{ii}$ | 0.95 | 2.59 | 3.097 (8) | 114 |
| C91—H91···O12$^{iii}$ | 0.95 | 2.33 | 3.227 (8) | 156 |
| C77—H77···O24$^{iv}$ | 1.00 | 2.29 | 3.264 (8) | 164 |
| C76—H76···O21$^{iv}$ | 0.95 | 2.50 | 3.399 (9) | 158 |
| C69—H69$A$···O14$^{v}$ | 0.98 | 2.44 | 3.323 (10) | 150 |
| C68—H68$A$···O10 | 0.98 | 2.55 | 3.214 (11) | 125 |
| C68—H68$A$···O9 | 0.98 | 2.66 | 3.224 (11) | 117 |
| C65—H65···O20$^{vi}$ | 0.95 | 2.64 | 3.485 (8) | 148 |
| C61—H61···O13$^{vi}$ | 0.95 | 2.49 | 3.429 (8) | 172 |
| C54—H54···O11$^{vi}$ | 1.00 | 2.30 | 3.277 (8) | 165 |
| C46—H46···O25 | 0.95 | 2.32 | 3.211 (8) | 155 |
| C46—H46···O8$^{i}$ | 0.95 | 2.56 | 3.054 (8) | 113 |
| C39—H39$A$···O27$^{i}$ | 0.98 | 2.54 | 3.338 (9) | 138 |
| N38—H38···O18 | 0.86 | 1.87 | 2.550 (6) | 135 |
| N33—H33···O4 | 0.86 | 1.87 | 2.545 (7) | 134 |
| N37—H37···O17 | 0.83 | 1.89 | 2.582 (7) | 139 |
| N32—H32···O5 | 1.04 | 1.71 | 2.578 (6) | 138 |

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

Intramolecular hydrogen bonds occur between the iminium protons and the phenolic oxygen atoms, with lengths of 1.71–1.89 Å (Table 1, Fig. 1). The bond distances and angles in the ligand are similar to those of analogous complexes (Hayashi *et al.*, 2013).

## 3. Supramolecular features

Though some weak C—H···O intermolecular interactions are found (Table 1), no strong interactions such as O—H···O hydrogen bonds between molecules are observed in the crystal. Hirshfeld surface analysis (Spackman *et al.*, 2009) was performed to investigate interactions in the crystal packing.

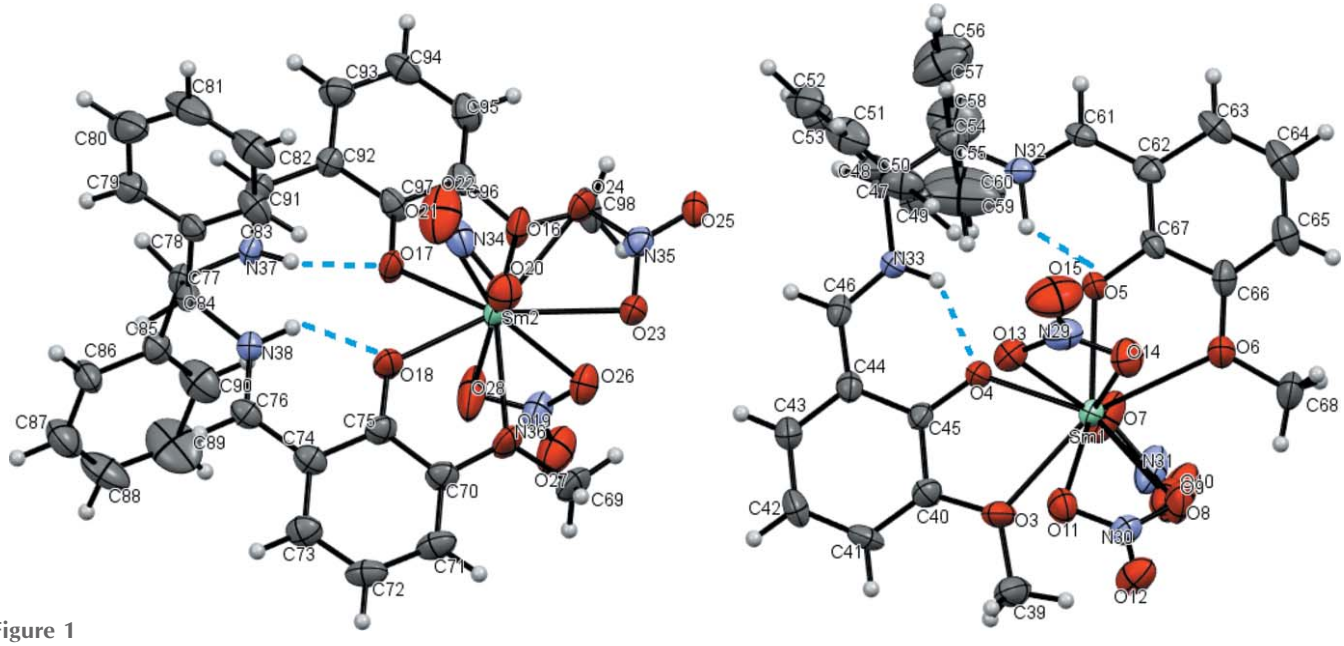



**Figure 1**
View of the two independent complex molecules of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines. **All non-H atoms should be labelled**

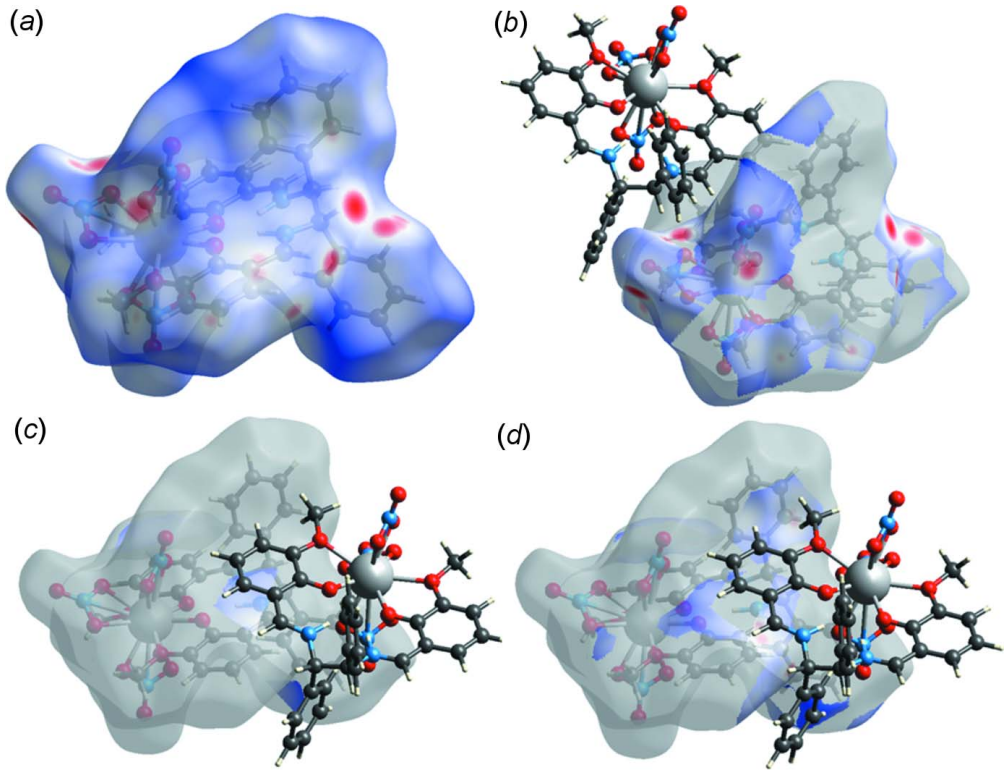



**Figure 2**
Hirshfeld surfaces plotted over of $d_{\mathrm{norm\ for}}$ (*a*) all interactions and (*b*) O···H/H···O, (*c*) C···C and (*d*) C···H/H···C contacts.

Hirshfeld surfaces and fingerprint plots (McKinnon *et al.*, 2004) were calculated using *CrystalExplorer17.5* (Turner *et al.*, 2017). Hydrogen bonds are strong interactions and they are indicated as red dots on the surface (Fig. 2) or two sharp spikes in the fingerprint plot (Fig. 3). 'Wings' in the fingerprint plots and diagonal plots at 1.8 Å are regarded as a characteristic feature potentially resulting from aromatic rings (Spackman *et al.*, 2002)The contributions to the Hirshfeld surface are H···H (33.5%), O···H (34.1%) and C···H (21.7%) contacts.

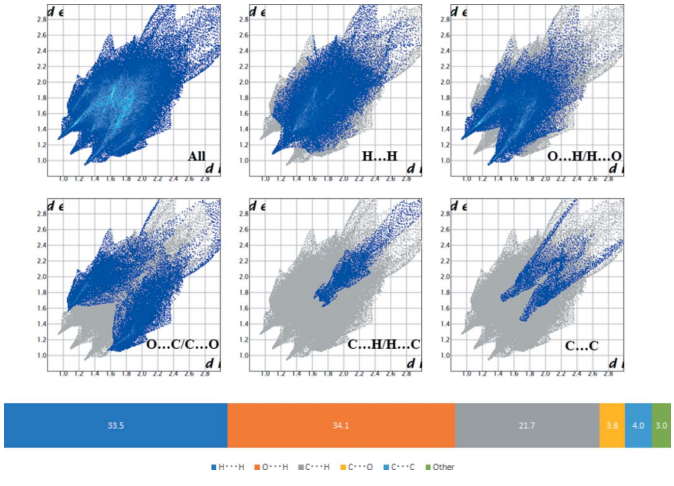



**Figure 3**
Two-dimensional fingerprint plots and contributions for various interactions.

## 4. Database survey

A search in the Cambridge Structural Database (CSD, Version 5.41, update of November 2019; Groom *et al.*, 2016) for similar structures returned two relevant entries: (*N*,*N*′-ethane-1,2-diylbis{[2-(oxy)-3-(methoxy)phenyl]methaniminiumato})tris(nitrato)samarium (refcode MOLNEI; Yang *et al.*, 2013) and (*S*,*S*)-{$\mu$-[2,2′-{(1,2-diphenylethane-1,2-diyl)bis[(azanylylidene)methylylidene]}bis[6-(methoxy)phenolato]]}trinitratoeuropium(III)nickel(II) (JIWNEL; Mayans *et al.*, 2019). In MOLNEI, a similar intramolecular N—H···O hydrogen bond is observed. Although the ligand of JIWNEL is similar to that in the title compound, the coordinating sites are filled with europium(III) and nickel(II) ions. For both MOLNEI and JIWNEL, the crystal packing is dominated by van der Waals interactions and C—H···O hydrogen bonds.

## 5. Synthesis and crystallization

(1*S*,2*S*)-(−)-1,2-Diphenylethylenediamine (0.100 g, 0.471 mmol) and *o*-vanillin (0.143 g, 0.940 mmol) were dissolved in ethanol (30 mL) and the resulting mixture was stirred at 313 K for 1 h to afford a yellow solution. To this solution, samarium nitrate hexahydrate (0.208 g, 0.468 mmol) was added and it was stirred at 313 K for 2 h. A yellow precipitate appeared immediately. The precipitate was filtered and washed with ethanol and hexane. The title compound (0.299 g, 0.366 mmol, yield 78.2%) was obtained as a yellow solid. IR (KBr, cm$^{-1}$) : 1624 (C=N double bond). Fluorescence bands in methanol solution were observed at 562

($^4G_{5/2} \rightarrow {}^6H_{5/2}$), 597 ($^4G_{5/2} \rightarrow {}^6H_{7/2}$) and 644 ($^4G_{5/2} \rightarrow {}^6H_{9/2}$) nm. Single crystals suitable for X-ray diffraction were obtained by recrystallization from methanol and diethyl ether (1:4, *v*/*v*) solution.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All C-bound H atoms were placed in geometrically calculated positions (C—H = 0.93–0.98 Å) and were constrained using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(C-methyl). SIMU, ISOR and AFIX 66 commands were used for C55, C56, C57, C58, C59, C60 to suppress temperature anisotropy and restrain bond lengths to appropriate values.


## Funding information

This work was supported by a Grant-in-Aid for Scientific Research (A) KAKENHI (20H00336).


**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Sm(NO_3)_3(C_{30}H_{28}N_2O_4)]$ |
| $M_r$ | 816.92 |
| Crystal system, space group | Monoclinic, *C*2 |
| Temperature (K) | 173 |
| *a*, *b*, *c* (Å) | 18.9105 (6), 15.7993 (5), 21.5738 (7) |
| $\beta$ (°) | 98.727 (1) |
| $V$ (Å$^3$) | 6371.0 (4) |
| $Z$ | 8 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.92 |
| Crystal size (mm) | 0.59 × 0.30 × 0.10 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXIII CCD |
| Absorption correction | Multi-scan |
| $T_{min}$, $T_{max}$ | 0.40, 0.83 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 40695, 15028, 12523 |
| $R_{int}$ | 0.042 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.732 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.033, 0.116, 0.83 |
| No. of reflections | 15028 |
| No. of parameters | 881 |
| No. of restraints | 49 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.84, −1.58 |
| Absolute structure | Flack *x* determined using 4865 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013) |
| Absolute structure parameter | 0.009 (9) |

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *shelXle* (Hübschle *et al.*, 2011) and *SHELXTL* (Sheldrick, 2008).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# supporting information

*Acta Cryst.* (2021). E**77**, 579-582 [https://doi.org/10.1107/S2056989021004424]

# Crystal structure and Hirshfeld surface analysis of ((*S*,*S*)-2,2′-{[(1,2-diphenylethane-1,2-diyl)bis[(azaniumylylidene)methanylylidene]}bis(6-methoxyphenolato))trinitratosamarium(III)

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## Computing details

Data collection: *APEX3* (Bruker, 2017); cell refinement: *APEX3* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015b); molecular graphics: *shelXle* (Hübschle *et al.*, 2011); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

**((*S*,*S*)-2,2′-{(1,2-diphenylethane-1,2-diyl)bis[(azaniumylylidene)methanylylidene]}bis(6-methoxyphenolato))trinitratosamarium(III)**

*Crystal data*

$[Sm(NO_3)_3(C_{30}H_{28}N_2O_4)]$
$M_r$ = 816.92
Monoclinic, *C*2
*a* = 18.9105 (6) Å
*b* = 15.7993 (5) Å
*c* = 21.5738 (7) Å
*β* = 98.727 (1)°
*V* = 6371.0 (4) Å$^3$
*Z* = 8
*F*(000) = 3272
$D_x$ = 1.703 Mg m$^{-3}$
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 859 reflections
*θ* = 1.7–28.6°
*μ* = 1.92 mm$^{-1}$
*T* = 173 K
Prism, yellow
0.59 × 0.30 × 0.10 mm

*Data collection*

Bruker APEXIII CCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 7.3910 pixels mm$^{-1}$
*φ* and *ω* scans
Absorption correction: multi-scan
$T_{min}$ = 0.40, $T_{max}$ = 0.83
40695 measured reflections
15028 independent reflections
12523 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042
$\theta_{max}$ = 31.3°, $\theta_{min}$ = 1.9°
*h* = −27→27
*k* = −20→21
*l* = −28→30

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.116
*S* = 0.83
15028 reflections
881 parameters
49 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.6514P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.84$ e Å$^{-3}$
$\Delta\rho_{min} = -1.58$ e Å$^{-3}$

Absolute structure: Flack *x* determined using 4865 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.009 (9)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sm1 | 0.34946 (2) | 0.59358 (2) | 0.63113 (2) | 0.03104 (10) |
| Sm2 | 0.34751 (2) | 0.39584 (2) | 0.13107 (2) | 0.03191 (11) |
| O3 | 0.4131 (3) | 0.4594 (4) | 0.5968 (2) | 0.0440 (13) |
| O4 | 0.3665 (2) | 0.5842 (4) | 0.52494 (19) | 0.0336 (10) |
| O5 | 0.3218 (3) | 0.7237 (3) | 0.5804 (2) | 0.0342 (11) |
| O6 | 0.3492 (3) | 0.7271 (4) | 0.7027 (2) | 0.0398 (12) |
| H32 | 0.312210 | 0.749766 | 0.502781 | 0.05 (2)* |
| O7 | 0.4735 (3) | 0.6447 (5) | 0.6256 (3) | 0.065 (2) |
| O9 | 0.4581 (3) | 0.5828 (6) | 0.7107 (2) | 0.0519 (16) |
| O8 | 0.5637 (3) | 0.6337 (7) | 0.7015 (3) | 0.081 (3) |
| O10 | 0.3289 (3) | 0.5319 (4) | 0.7402 (2) | 0.0497 (14) |
| O11 | 0.2958 (3) | 0.4561 (4) | 0.6585 (2) | 0.0401 (12) |
| O12 | 0.2771 (3) | 0.4098 (5) | 0.7490 (2) | 0.0501 (16) |
| O13 | 0.2293 (3) | 0.5689 (4) | 0.5608 (2) | 0.0416 (13) |
| O14 | 0.2255 (3) | 0.6244 (4) | 0.6515 (2) | 0.0509 (15) |
| O15 | 0.1278 (3) | 0.6161 (6) | 0.5828 (4) | 0.081 (3) |
| O16 | 0.4178 (3) | 0.5280 (4) | 0.0995 (2) | 0.0423 (13) |
| O17 | 0.3733 (2) | 0.4025 (4) | 0.02689 (18) | 0.0361 (11) |
| O18 | 0.3128 (3) | 0.2709 (3) | 0.0773 (2) | 0.0392 (11) |
| O19 | 0.3455 (3) | 0.2594 (4) | 0.1986 (2) | 0.0449 (13) |
| O20 | 0.2196 (3) | 0.3731 (4) | 0.1473 (2) | 0.0473 (13) |
| O21 | 0.2315 (3) | 0.4286 (4) | 0.0572 (2) | 0.0438 (14) |
| O22 | 0.1272 (3) | 0.3899 (7) | 0.0772 (3) | 0.082 (2) |
| O23 | 0.3243 (3) | 0.4607 (3) | 0.2386 (2) | 0.0399 (12) |
| H37 | 0.336816 | 0.342349 | −0.046833 | 0.06 (2)* |
| O24 | 0.2953 (3) | 0.5368 (4) | 0.1565 (2) | 0.0407 (13) |
| O25 | 0.2780 (2) | 0.5849 (4) | 0.24702 (19) | 0.0387 (11) |
| O26 | 0.4537 (3) | 0.4042 (5) | 0.2154 (2) | 0.0456 (13) |
| O27 | 0.5601 (3) | 0.3585 (5) | 0.2082 (2) | 0.0656 (19) |
| O28 | 0.4709 (3) | 0.3425 (6) | 0.1312 (3) | 0.074 (2) |
| N29 | 0.1918 (3) | 0.6040 (6) | 0.5969 (3) | 0.0446 (17) |
| N30 | 0.3004 (3) | 0.4638 (5) | 0.7169 (3) | 0.0369 (15) |
| N31 | 0.5005 (3) | 0.6206 (7) | 0.6799 (3) | 0.059 (3) |
| N32 | 0.3003 (2) | 0.8029 (3) | 0.4747 (2) | 0.0295 (10) |

| | | | | |
|---|---|---|---|---|
| N33 | 0.3249 (3) | 0.6451 (4) | 0.4163 (2) | 0.0274 (10) |
| H33 | 0.330349 | 0.652121 | 0.456298 | 0.033* |
| N34 | 0.1893 (3) | 0.3978 (6) | 0.0936 (3) | 0.0458 (15) |
| N35 | 0.2982 (3) | 0.5279 (4) | 0.2156 (2) | 0.0334 (14) |
| N36 | 0.4974 (3) | 0.3681 (5) | 0.1853 (3) | 0.0427 (18) |
| N37 | 0.3445 (3) | 0.3371 (4) | −0.0837 (2) | 0.0290 (11) |
| N38 | 0.2753 (2) | 0.2045 (3) | −0.0304 (2) | 0.0283 (10) |
| H38 | 0.281783 | 0.249361 | −0.007628 | 0.034* |
| C39 | 0.4367 (4) | 0.3910 (7) | 0.6385 (3) | 0.051 (2) |
| H39A | 0.445994 | 0.412274 | 0.681699 | 0.077* |
| H39B | 0.480660 | 0.366718 | 0.627254 | 0.077* |
| H39C | 0.399464 | 0.347401 | 0.635258 | 0.077* |
| C40 | 0.4033 (4) | 0.4420 (5) | 0.5336 (3) | 0.0346 (17) |
| C41 | 0.4114 (3) | 0.3647 (4) | 0.5056 (3) | 0.0370 (17) |
| H41 | 0.425050 | 0.316532 | 0.530957 | 0.044* |
| C42 | 0.3999 (4) | 0.3567 (5) | 0.4409 (3) | 0.0450 (18) |
| H42 | 0.404084 | 0.303086 | 0.421899 | 0.054* |
| C43 | 0.3821 (4) | 0.4278 (5) | 0.4040 (3) | 0.0390 (17) |
| H43 | 0.377368 | 0.423280 | 0.359672 | 0.047* |
| C44 | 0.3710 (3) | 0.5060 (5) | 0.4313 (3) | 0.0306 (14) |
| C45 | 0.3808 (3) | 0.5142 (5) | 0.4972 (3) | 0.0261 (13) |
| C46 | 0.3426 (3) | 0.5731 (5) | 0.3933 (3) | 0.0287 (15) |
| H46 | 0.336029 | 0.566135 | 0.349023 | 0.034* |
| C47 | 0.2838 (3) | 0.7123 (4) | 0.3798 (2) | 0.0294 (11) |
| H47 | 0.296223 | 0.710575 | 0.336410 | 0.035* |
| C48 | 0.2038 (3) | 0.6939 (4) | 0.3748 (3) | 0.0314 (13) |
| C49 | 0.1730 (3) | 0.6685 (5) | 0.4268 (3) | 0.0353 (14) |
| H49 | 0.201824 | 0.663385 | 0.466731 | 0.042* |
| C50 | 0.1002 (4) | 0.6509 (5) | 0.4202 (4) | 0.0455 (18) |
| H50 | 0.079376 | 0.633347 | 0.455476 | 0.055* |
| C51 | 0.0585 (4) | 0.6587 (5) | 0.3627 (4) | 0.051 (2) |
| H51 | 0.008972 | 0.645444 | 0.358318 | 0.062* |
| C53 | 0.1603 (4) | 0.7029 (5) | 0.3165 (3) | 0.0361 (15) |
| H53 | 0.180623 | 0.720595 | 0.280987 | 0.043* |
| C52 | 0.0877 (4) | 0.6858 (6) | 0.3107 (4) | 0.0477 (18) |
| H52 | 0.058045 | 0.692689 | 0.271375 | 0.057* |
| C54 | 0.3039 (3) | 0.8011 (4) | 0.4069 (2) | 0.0307 (11) |
| H54 | 0.266389 | 0.840983 | 0.386531 | 0.037* |
| C55 | 0.37537 (19) | 0.8350 (3) | 0.3938 (3) | 0.0392 (13) |
| C56 | 0.3759 (2) | 0.9062 (4) | 0.3560 (3) | 0.069 (2) |
| H56 | 0.332134 | 0.931450 | 0.337664 | 0.083* |
| C57 | 0.4406 (3) | 0.9405 (4) | 0.3451 (3) | 0.079 (3) |
| H57 | 0.441010 | 0.989164 | 0.319282 | 0.095* |
| C58 | 0.5047 (2) | 0.9036 (5) | 0.3720 (4) | 0.073 (2) |
| H58 | 0.548925 | 0.927044 | 0.364509 | 0.087* |
| C59 | 0.50415 (19) | 0.8324 (5) | 0.4098 (4) | 0.118 (4) |
| H59 | 0.547964 | 0.807212 | 0.428118 | 0.141* |
| C60 | 0.4395 (2) | 0.7981 (4) | 0.4207 (3) | 0.106 (3) |

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|---|---|---|---|---|
| H60 | 0.439088 | 0.749498 | 0.446501 | 0.128* |
| C61 | 0.2952 (3) | 0.8720 (4) | 0.5059 (3) | 0.0283 (12) |
| H61 | 0.285957 | 0.923758 | 0.483751 | 0.034* |
| C62 | 0.3030 (3) | 0.8722 (5) | 0.5719 (3) | 0.0312 (15) |
| C63 | 0.3003 (4) | 0.9513 (5) | 0.6042 (4) | 0.0373 (16) |
| H63 | 0.290380 | 1.002088 | 0.580941 | 0.045* |
| C64 | 0.3119 (4) | 0.9538 (6) | 0.6681 (4) | 0.0469 (19) |
| H64 | 0.309507 | 1.006212 | 0.689194 | 0.056* |
| C65 | 0.3274 (4) | 0.8795 (5) | 0.7026 (3) | 0.0397 (17) |
| H65 | 0.334973 | 0.882498 | 0.747141 | 0.048* |
| C66 | 0.3318 (4) | 0.8029 (5) | 0.6744 (3) | 0.0354 (15) |
| C67 | 0.3177 (3) | 0.7977 (5) | 0.6067 (3) | 0.0281 (14) |
| C68 | 0.3680 (4) | 0.7271 (6) | 0.7700 (3) | 0.0499 (19) |
| H68A | 0.384219 | 0.670427 | 0.784231 | 0.075* |
| H68B | 0.326080 | 0.742748 | 0.789153 | 0.075* |
| H68C | 0.406501 | 0.768006 | 0.782367 | 0.075* |
| C69 | 0.3627 (5) | 0.2536 (6) | 0.2657 (3) | 0.057 (2) |
| H69A | 0.322245 | 0.228728 | 0.282772 | 0.085* |
| H69B | 0.372451 | 0.310348 | 0.283318 | 0.085* |
| H69C | 0.405073 | 0.217886 | 0.276765 | 0.085* |
| C70 | 0.3310 (4) | 0.1831 (5) | 0.1664 (3) | 0.0342 (15) |
| C71 | 0.3305 (4) | 0.1039 (6) | 0.1932 (3) | 0.0419 (17) |
| H71 | 0.338944 | 0.097875 | 0.237482 | 0.050* |
| C72 | 0.3176 (4) | 0.0323 (5) | 0.1545 (4) | 0.0423 (17) |
| H72 | 0.318484 | −0.022487 | 0.172839 | 0.051* |
| C73 | 0.3036 (4) | 0.0408 (5) | 0.0901 (3) | 0.0387 (16) |
| H73 | 0.296486 | −0.008063 | 0.064178 | 0.046* |
| C74 | 0.3000 (3) | 0.1208 (5) | 0.0631 (3) | 0.0323 (16) |
| C75 | 0.3144 (4) | 0.1955 (5) | 0.1012 (3) | 0.0326 (15) |
| C76 | 0.2819 (3) | 0.1313 (4) | −0.0040 (3) | 0.0307 (13) |
| H76 | 0.274596 | 0.082215 | −0.029571 | 0.037* |
| C77 | 0.2589 (3) | 0.2203 (3) | −0.0980 (2) | 0.0289 (10) |
| H77 | 0.251341 | 0.164019 | −0.119107 | 0.035* |
| C78 | 0.1892 (3) | 0.2715 (4) | −0.1156 (3) | 0.0320 (13) |
| C79 | 0.1580 (5) | 0.2715 (5) | −0.1764 (4) | 0.0464 (19) |
| H79 | 0.181222 | 0.243622 | −0.206714 | 0.056* |
| C80 | 0.0928 (5) | 0.3114 (6) | −0.1954 (4) | 0.062 (2) |
| H80 | 0.072411 | 0.311722 | −0.238458 | 0.074* |
| C81 | 0.0583 (4) | 0.3498 (6) | −0.1523 (5) | 0.064 (3) |
| H81 | 0.012808 | 0.375385 | −0.164474 | 0.077* |
| C82 | 0.0911 (4) | 0.3511 (6) | −0.0897 (5) | 0.057 (2) |
| H82 | 0.059 (4) | 0.370 (6) | −0.064 (4) | 0.06 (2)* |
| C83 | 0.1553 (4) | 0.3129 (5) | −0.0719 (4) | 0.0423 (16) |
| H83 | 0.176979 | 0.314561 | −0.029180 | 0.051* |
| C84 | 0.3251 (3) | 0.2616 (4) | −0.1208 (2) | 0.0329 (11) |
| H84 | 0.311382 | 0.278765 | −0.165589 | 0.039* |
| C86 | 0.3769 (3) | 0.1272 (4) | −0.1558 (3) | 0.0393 (14) |
| H86 | 0.333439 | 0.119803 | −0.183756 | 0.047* |

| | | | | |
|---|---|---|---|---|
| C85 | 0.3858 (3) | 0.1973 (4) | −0.1169 (3) | 0.0322 (11) |
| C87 | 0.4309 (4) | 0.0681 (6) | −0.1540 (4) | 0.0556 (19) |
| H87 | 0.422910 | 0.019203 | −0.179743 | 0.067* |
| C89 | 0.5036 (4) | 0.1445 (7) | −0.0774 (5) | 0.088 (4) |
| H89 | 0.546499 | 0.149087 | −0.048387 | 0.106* |
| C88 | 0.4945 (4) | 0.0776 (6) | −0.1170 (5) | 0.063 (2) |
| H88 | 0.532161 | 0.038266 | −0.118688 | 0.076* |
| C90 | 0.4500 (4) | 0.2080 (5) | −0.0785 (4) | 0.0558 (18) |
| H90 | 0.458592 | 0.257054 | −0.052928 | 0.067* |
| C91 | 0.3504 (3) | 0.4121 (5) | −0.1058 (3) | 0.0297 (14) |
| H91 | 0.341392 | 0.419984 | −0.149996 | 0.036* |
| C92 | 0.3701 (3) | 0.4843 (5) | −0.0666 (3) | 0.0269 (13) |
| C93 | 0.3750 (4) | 0.5661 (5) | −0.0934 (4) | 0.0389 (17) |
| H93 | 0.364489 | 0.573123 | −0.137529 | 0.047* |
| C94 | 0.3946 (4) | 0.6338 (5) | −0.0564 (4) | 0.0402 (16) |
| H94 | 0.397898 | 0.687958 | −0.074857 | 0.048* |
| C95 | 0.4104 (4) | 0.6247 (5) | 0.0098 (3) | 0.0403 (19) |
| H95 | 0.424791 | 0.672383 | 0.035450 | 0.048* |
| C96 | 0.4046 (3) | 0.5466 (5) | 0.0363 (3) | 0.0302 (15) |
| C97 | 0.3825 (3) | 0.4752 (5) | −0.0004 (3) | 0.0324 (15) |
| C98 | 0.4469 (4) | 0.5942 (7) | 0.1414 (3) | 0.0467 (18) |
| H98A | 0.456507 | 0.572119 | 0.184323 | 0.070* |
| H98B | 0.412560 | 0.640895 | 0.139544 | 0.070* |
| H98C | 0.491636 | 0.614798 | 0.129001 | 0.070* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sm1 | 0.0435 (2) | 0.0290 (2) | 0.02008 (18) | 0.00589 (17) | 0.00313 (14) | −0.00049 (14) |
| Sm2 | 0.0474 (2) | 0.0301 (2) | 0.01812 (17) | −0.00325 (17) | 0.00465 (15) | −0.00037 (14) |
| O3 | 0.064 (3) | 0.034 (3) | 0.036 (3) | 0.019 (3) | 0.013 (2) | 0.010 (2) |
| O4 | 0.050 (2) | 0.028 (3) | 0.0227 (19) | 0.010 (2) | 0.0059 (17) | 0.001 (2) |
| O5 | 0.054 (3) | 0.024 (2) | 0.024 (2) | 0.005 (2) | 0.0048 (18) | −0.0034 (19) |
| O6 | 0.059 (3) | 0.033 (3) | 0.028 (2) | 0.002 (3) | 0.005 (2) | −0.004 (2) |
| O7 | 0.054 (3) | 0.107 (6) | 0.033 (3) | −0.017 (4) | 0.004 (2) | 0.002 (3) |
| O9 | 0.048 (3) | 0.071 (5) | 0.034 (2) | 0.010 (3) | −0.001 (2) | 0.004 (3) |
| O8 | 0.042 (3) | 0.157 (8) | 0.044 (3) | 0.005 (4) | 0.000 (2) | −0.007 (4) |
| O10 | 0.072 (3) | 0.044 (3) | 0.031 (3) | −0.018 (3) | 0.001 (2) | −0.011 (3) |
| O11 | 0.048 (3) | 0.036 (3) | 0.036 (3) | −0.004 (2) | 0.005 (2) | −0.007 (2) |
| O12 | 0.052 (3) | 0.052 (4) | 0.043 (3) | −0.018 (3) | −0.004 (2) | 0.011 (3) |
| O13 | 0.050 (3) | 0.042 (3) | 0.032 (2) | 0.004 (2) | 0.003 (2) | 0.004 (2) |
| O14 | 0.061 (3) | 0.056 (4) | 0.038 (3) | 0.012 (3) | 0.016 (2) | −0.005 (3) |
| O15 | 0.052 (3) | 0.096 (6) | 0.093 (5) | 0.019 (4) | 0.009 (3) | 0.024 (5) |
| O16 | 0.057 (3) | 0.050 (4) | 0.021 (2) | −0.014 (3) | 0.007 (2) | −0.009 (2) |
| O17 | 0.060 (3) | 0.029 (3) | 0.0190 (19) | −0.009 (3) | 0.0066 (18) | −0.001 (2) |
| O18 | 0.064 (3) | 0.029 (3) | 0.026 (2) | −0.005 (2) | 0.007 (2) | 0.004 (2) |
| O19 | 0.076 (3) | 0.038 (3) | 0.020 (2) | −0.007 (3) | 0.004 (2) | 0.007 (2) |
| O20 | 0.053 (3) | 0.049 (3) | 0.042 (3) | −0.008 (3) | 0.012 (2) | 0.001 (2) |

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|---|---|---|---|---|---|---|
| O21 | 0.054 (3) | 0.049 (3) | 0.026 (2) | 0.003 (3) | −0.001 (2) | 0.004 (2) |
| O22 | 0.043 (3) | 0.126 (7) | 0.074 (4) | −0.004 (4) | 0.001 (3) | −0.025 (5) |
| O23 | 0.061 (3) | 0.033 (3) | 0.024 (2) | 0.005 (3) | 0.001 (2) | −0.001 (2) |
| O24 | 0.068 (3) | 0.036 (3) | 0.019 (2) | −0.001 (3) | 0.011 (2) | 0.004 (2) |
| O25 | 0.049 (2) | 0.040 (3) | 0.027 (2) | −0.001 (3) | 0.0064 (18) | −0.009 (2) |
| O26 | 0.053 (3) | 0.057 (4) | 0.028 (2) | −0.002 (3) | 0.010 (2) | −0.006 (3) |
| O27 | 0.053 (3) | 0.101 (6) | 0.044 (3) | 0.007 (3) | 0.009 (2) | −0.003 (3) |
| O28 | 0.063 (4) | 0.119 (7) | 0.038 (3) | 0.014 (4) | 0.000 (3) | −0.035 (4) |
| N29 | 0.041 (3) | 0.046 (4) | 0.047 (4) | 0.008 (3) | 0.006 (3) | 0.010 (3) |
| N30 | 0.046 (3) | 0.037 (4) | 0.028 (3) | 0.000 (3) | 0.005 (2) | 0.006 (3) |
| N31 | 0.039 (3) | 0.099 (8) | 0.037 (3) | 0.007 (4) | 0.002 (3) | −0.011 (4) |
| N32 | 0.030 (2) | 0.025 (3) | 0.032 (2) | 0.002 (2) | 0.0013 (18) | 0.0037 (18) |
| N33 | 0.032 (2) | 0.027 (3) | 0.024 (2) | 0.003 (2) | 0.0046 (18) | 0.0007 (19) |
| N34 | 0.048 (3) | 0.042 (4) | 0.047 (4) | −0.001 (3) | 0.007 (3) | −0.016 (3) |
| N35 | 0.034 (3) | 0.034 (4) | 0.029 (3) | −0.004 (3) | −0.002 (2) | 0.001 (3) |
| N36 | 0.046 (3) | 0.055 (5) | 0.028 (3) | 0.000 (3) | 0.005 (2) | −0.004 (3) |
| N37 | 0.034 (2) | 0.034 (3) | 0.018 (2) | 0.001 (2) | 0.0028 (18) | −0.0017 (19) |
| N38 | 0.033 (2) | 0.028 (2) | 0.024 (2) | 0.001 (2) | 0.0035 (17) | −0.0024 (18) |
| C39 | 0.071 (5) | 0.048 (5) | 0.037 (4) | 0.022 (5) | 0.015 (3) | 0.012 (4) |
| C40 | 0.045 (4) | 0.031 (4) | 0.029 (3) | 0.003 (3) | 0.010 (3) | 0.004 (3) |
| C41 | 0.042 (3) | 0.019 (4) | 0.052 (4) | 0.009 (3) | 0.014 (3) | 0.006 (3) |
| C42 | 0.059 (4) | 0.037 (4) | 0.039 (4) | 0.005 (4) | 0.008 (3) | −0.017 (3) |
| C43 | 0.050 (4) | 0.036 (4) | 0.029 (3) | 0.007 (3) | 0.001 (3) | −0.007 (3) |
| C44 | 0.029 (3) | 0.035 (4) | 0.027 (3) | 0.002 (3) | 0.002 (2) | −0.006 (3) |
| C45 | 0.026 (3) | 0.031 (4) | 0.021 (3) | 0.003 (3) | 0.000 (2) | −0.001 (3) |
| C46 | 0.027 (3) | 0.037 (4) | 0.022 (3) | −0.001 (3) | 0.001 (2) | −0.005 (3) |
| C47 | 0.038 (3) | 0.030 (3) | 0.021 (2) | 0.002 (2) | 0.005 (2) | 0.004 (2) |
| C48 | 0.031 (3) | 0.024 (3) | 0.036 (3) | 0.004 (2) | −0.004 (2) | 0.003 (2) |
| C49 | 0.034 (3) | 0.032 (3) | 0.038 (3) | −0.006 (3) | −0.002 (2) | 0.003 (3) |
| C50 | 0.039 (3) | 0.036 (4) | 0.062 (4) | −0.004 (3) | 0.010 (3) | 0.011 (3) |
| C51 | 0.029 (3) | 0.037 (4) | 0.083 (6) | −0.008 (3) | −0.008 (3) | −0.005 (4) |
| C53 | 0.042 (3) | 0.033 (4) | 0.030 (3) | 0.007 (3) | −0.004 (2) | −0.001 (3) |
| C52 | 0.040 (3) | 0.041 (4) | 0.054 (4) | −0.005 (3) | −0.018 (3) | 0.000 (4) |
| C54 | 0.033 (2) | 0.030 (3) | 0.029 (2) | −0.002 (2) | 0.005 (2) | 0.003 (2) |
| C55 | 0.027 (2) | 0.036 (3) | 0.055 (3) | −0.002 (3) | 0.009 (2) | 0.002 (3) |
| C56 | 0.048 (4) | 0.084 (6) | 0.070 (5) | −0.020 (4) | −0.005 (3) | 0.038 (4) |
| C57 | 0.050 (4) | 0.092 (6) | 0.093 (6) | −0.036 (4) | 0.003 (4) | 0.032 (5) |
| C58 | 0.040 (3) | 0.076 (6) | 0.106 (6) | −0.009 (4) | 0.024 (4) | 0.010 (5) |
| C59 | 0.044 (4) | 0.087 (7) | 0.223 (9) | −0.007 (5) | 0.020 (6) | 0.060 (7) |
| C60 | 0.039 (4) | 0.076 (6) | 0.202 (8) | −0.005 (4) | 0.012 (5) | 0.065 (6) |
| C61 | 0.026 (2) | 0.021 (3) | 0.038 (3) | 0.006 (2) | 0.003 (2) | 0.002 (2) |
| C62 | 0.023 (3) | 0.031 (4) | 0.039 (3) | 0.006 (3) | 0.004 (2) | −0.001 (3) |
| C63 | 0.037 (3) | 0.022 (3) | 0.055 (4) | 0.004 (3) | 0.014 (3) | −0.009 (3) |
| C64 | 0.047 (4) | 0.035 (4) | 0.061 (5) | 0.001 (3) | 0.016 (3) | −0.020 (3) |
| C65 | 0.042 (3) | 0.041 (4) | 0.040 (3) | −0.005 (3) | 0.017 (3) | −0.014 (3) |
| C66 | 0.042 (3) | 0.041 (4) | 0.025 (3) | −0.001 (3) | 0.010 (3) | −0.009 (3) |
| C67 | 0.028 (3) | 0.023 (3) | 0.034 (3) | 0.004 (3) | 0.005 (2) | −0.009 (3) |
| C68 | 0.076 (5) | 0.046 (4) | 0.026 (3) | −0.004 (4) | 0.001 (3) | −0.008 (3) |

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|---|---|---|---|---|---|---|
| C69 | 0.093 (6) | 0.050 (5) | 0.025 (3) | −0.001 (5) | 0.001 (4) | 0.011 (3) |
| C70 | 0.039 (3) | 0.028 (4) | 0.035 (3) | −0.006 (3) | 0.006 (3) | 0.006 (3) |
| C71 | 0.043 (3) | 0.039 (4) | 0.043 (4) | −0.004 (3) | 0.002 (3) | 0.017 (3) |
| C72 | 0.039 (3) | 0.032 (4) | 0.054 (4) | −0.001 (3) | 0.001 (3) | 0.016 (3) |
| C73 | 0.039 (3) | 0.033 (4) | 0.043 (4) | −0.007 (3) | 0.006 (3) | 0.006 (3) |
| C74 | 0.030 (3) | 0.027 (4) | 0.040 (3) | −0.004 (3) | 0.009 (3) | 0.001 (3) |
| C75 | 0.038 (3) | 0.033 (4) | 0.029 (3) | 0.001 (3) | 0.011 (2) | 0.008 (3) |
| C76 | 0.029 (2) | 0.025 (3) | 0.040 (3) | −0.003 (2) | 0.009 (2) | −0.001 (2) |
| C77 | 0.034 (3) | 0.026 (3) | 0.025 (2) | 0.001 (2) | −0.0019 (19) | −0.0051 (19) |
| C78 | 0.035 (3) | 0.021 (3) | 0.038 (3) | 0.000 (3) | −0.003 (2) | −0.006 (2) |
| C79 | 0.053 (4) | 0.034 (4) | 0.048 (4) | 0.005 (3) | −0.005 (3) | −0.002 (3) |
| C80 | 0.066 (5) | 0.038 (5) | 0.069 (5) | 0.002 (4) | −0.029 (4) | −0.002 (4) |
| C81 | 0.046 (4) | 0.031 (4) | 0.104 (7) | 0.010 (3) | −0.023 (4) | −0.011 (4) |
| C82 | 0.048 (4) | 0.033 (4) | 0.089 (6) | 0.001 (3) | 0.011 (4) | −0.014 (4) |
| C83 | 0.045 (3) | 0.029 (3) | 0.053 (4) | −0.004 (3) | 0.009 (3) | −0.011 (3) |
| C84 | 0.045 (3) | 0.033 (3) | 0.021 (2) | 0.000 (3) | 0.006 (2) | −0.003 (2) |
| C86 | 0.040 (3) | 0.033 (3) | 0.043 (3) | 0.006 (3) | −0.001 (2) | −0.013 (3) |
| C85 | 0.036 (3) | 0.032 (3) | 0.031 (3) | −0.001 (2) | 0.013 (2) | 0.000 (2) |
| C87 | 0.061 (4) | 0.043 (4) | 0.064 (5) | 0.011 (4) | 0.013 (4) | −0.014 (4) |
| C89 | 0.022 (3) | 0.095 (8) | 0.143 (9) | 0.004 (4) | −0.004 (4) | −0.027 (7) |
| C88 | 0.048 (4) | 0.040 (4) | 0.105 (7) | 0.012 (4) | 0.023 (4) | −0.005 (5) |
| C90 | 0.041 (3) | 0.047 (4) | 0.080 (5) | −0.006 (3) | 0.010 (3) | −0.011 (4) |
| C91 | 0.033 (3) | 0.031 (4) | 0.025 (3) | 0.000 (3) | 0.005 (2) | 0.000 (3) |
| C92 | 0.026 (3) | 0.029 (3) | 0.026 (3) | −0.003 (3) | 0.004 (2) | 0.000 (3) |
| C93 | 0.042 (4) | 0.031 (4) | 0.043 (4) | −0.001 (3) | 0.003 (3) | 0.006 (3) |
| C94 | 0.044 (4) | 0.023 (3) | 0.054 (4) | −0.005 (3) | 0.008 (3) | −0.003 (3) |
| C95 | 0.042 (4) | 0.037 (5) | 0.043 (4) | −0.010 (3) | 0.012 (3) | −0.009 (3) |
| C96 | 0.028 (3) | 0.030 (4) | 0.033 (3) | −0.005 (3) | 0.006 (3) | −0.004 (3) |
| C97 | 0.038 (3) | 0.024 (4) | 0.038 (4) | −0.006 (3) | 0.015 (3) | −0.006 (3) |
| C98 | 0.050 (3) | 0.045 (4) | 0.046 (4) | −0.013 (4) | 0.009 (3) | −0.024 (4) |

*Geometric parameters (Å, º)*

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| Sm1—O5 | 2.350 (5) | C50—H50 | 0.9500 |
| Sm1—O4 | 2.366 (4) | C51—C52 | 1.392 (11) |
| Sm1—O9 | 2.476 (5) | C51—H51 | 0.9500 |
| Sm1—O14 | 2.498 (5) | C53—C52 | 1.386 (10) |
| Sm1—O7 | 2.500 (6) | C53—H53 | 0.9500 |
| Sm1—O11 | 2.505 (6) | C52—H52 | 0.9500 |
| Sm1—O13 | 2.563 (5) | C54—C55 | 1.520 (6) |
| Sm1—O3 | 2.601 (5) | C54—H54 | 1.0000 |
| Sm1—O6 | 2.614 (5) | C55—C56 | 1.3900 |
| Sm1—O10 | 2.630 (5) | C55—C60 | 1.3900 |
| Sm1—N31 | 2.922 (6) | C56—C57 | 1.3900 |
| Sm1—N29 | 2.965 (6) | C56—H56 | 0.9500 |
| Sm2—O18 | 2.333 (5) | C57—C58 | 1.3900 |
| Sm2—O17 | 2.373 (4) | C57—H57 | 0.9500 |
| Sm2—O28 | 2.481 (6) | C58—C59 | 1.3900 |

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| Sm2—O26 | 2.500 (5) | C58—H58 | 0.9500 |
| Sm2—O20 | 2.522 (5) | C59—C60 | 1.3900 |
| Sm2—O24 | 2.530 (6) | C59—H59 | 0.9500 |
| Sm2—O21 | 2.561 (5) | C60—H60 | 0.9500 |
| Sm2—O19 | 2.606 (5) | C61—C62 | 1.409 (9) |
| Sm2—O16 | 2.621 (6) | C61—H61 | 0.9500 |
| Sm2—O23 | 2.634 (4) | C62—C67 | 1.402 (10) |
| Sm2—N36 | 2.930 (6) | C62—C63 | 1.435 (10) |
| Sm2—N34 | 2.978 (6) | C63—C64 | 1.363 (11) |
| O3—C40 | 1.375 (8) | C63—H63 | 0.9500 |
| O3—C39 | 1.433 (10) | C64—C65 | 1.397 (12) |
| O4—C45 | 1.304 (8) | C64—H64 | 0.9500 |
| O5—C67 | 1.306 (8) | C65—C66 | 1.363 (11) |
| O6—C66 | 1.362 (10) | C65—H65 | 0.9500 |
| O6—C68 | 1.442 (7) | C66—C67 | 1.447 (9) |
| O7—N31 | 1.263 (9) | C68—H68A | 0.9800 |
| O9—N31 | 1.267 (10) | C68—H68B | 0.9800 |
| O8—N31 | 1.232 (8) | C68—H68C | 0.9800 |
| O10—N30 | 1.272 (9) | C69—H69A | 0.9800 |
| O11—N30 | 1.255 (7) | C69—H69B | 0.9800 |
| O12—N30 | 1.223 (8) | C69—H69C | 0.9800 |
| O13—N29 | 1.259 (8) | C70—C71 | 1.378 (11) |
| O14—N29 | 1.291 (9) | C70—C75 | 1.408 (10) |
| O15—N29 | 1.219 (9) | C71—C72 | 1.406 (12) |
| O16—C96 | 1.380 (8) | C71—H71 | 0.9500 |
| O16—C98 | 1.437 (10) | C72—C73 | 1.382 (11) |
| O17—C97 | 1.315 (9) | C72—H72 | 0.9500 |
| O18—C75 | 1.295 (9) | C73—C74 | 1.389 (11) |
| O19—C70 | 1.397 (9) | C73—H73 | 0.9500 |
| O19—C69 | 1.438 (7) | C74—C75 | 1.439 (11) |
| O20—N34 | 1.273 (9) | C74—C76 | 1.445 (9) |
| O21—N34 | 1.296 (9) | C76—H76 | 0.9500 |
| O22—N34 | 1.181 (8) | C77—C78 | 1.544 (8) |
| O23—N35 | 1.241 (8) | C77—C84 | 1.555 (7) |
| O24—N35 | 1.278 (7) | C77—H77 | 1.0000 |
| O25—N35 | 1.222 (8) | C78—C79 | 1.353 (10) |
| O26—N36 | 1.260 (8) | C78—C83 | 1.383 (9) |
| O27—N36 | 1.223 (8) | C79—C80 | 1.391 (12) |
| O28—N36 | 1.265 (8) | C79—H79 | 0.9500 |
| N32—C61 | 1.292 (8) | C80—C81 | 1.357 (12) |
| N32—C54 | 1.475 (6) | C80—H80 | 0.9500 |
| N32—H32 | 1.0395 | C81—C82 | 1.399 (14) |
| N33—C46 | 1.305 (9) | C81—H81 | 0.9500 |
| N33—C47 | 1.473 (7) | C82—C83 | 1.358 (11) |
| N33—H33 | 0.8600 | C82—H82 | 0.92 (8) |
| N37—C91 | 1.290 (9) | C83—H83 | 0.9500 |
| N37—C84 | 1.451 (8) | C84—C85 | 1.526 (8) |
| N37—H37 | 0.8345 | C84—H84 | 1.0000 |

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| N38—C76 | 1.287 (8) | C86—C87 | 1.380 (10) |
| N38—C77 | 1.466 (6) | C86—C85 | 1.383 (8) |
| N38—H38 | 0.8600 | C86—H86 | 0.9500 |
| C39—H39A | 0.9800 | C85—C90 | 1.374 (9) |
| C39—H39B | 0.9800 | C87—C88 | 1.349 (12) |
| C39—H39C | 0.9800 | C87—H87 | 0.9500 |
| C40—C41 | 1.381 (10) | C89—C88 | 1.352 (13) |
| C40—C45 | 1.414 (10) | C89—C90 | 1.424 (12) |
| C41—C42 | 1.386 (9) | C89—H89 | 0.9500 |
| C41—H41 | 0.9500 | C88—H88 | 0.9500 |
| C42—C43 | 1.387 (12) | C90—H90 | 0.9500 |
| C42—H42 | 0.9500 | C91—C92 | 1.436 (10) |
| C43—C44 | 1.397 (11) | C91—H91 | 0.9500 |
| C43—H43 | 0.9500 | C92—C97 | 1.420 (9) |
| C44—C46 | 1.397 (11) | C92—C93 | 1.424 (11) |
| C44—C45 | 1.413 (8) | C93—C94 | 1.352 (11) |
| C46—H46 | 0.9500 | C93—H93 | 0.9500 |
| C47—C48 | 1.527 (8) | C94—C95 | 1.421 (10) |
| C47—C54 | 1.545 (8) | C94—H94 | 0.9500 |
| C47—H47 | 1.0000 | C95—C96 | 1.371 (11) |
| C48—C49 | 1.399 (9) | C95—H95 | 0.9500 |
| C48—C53 | 1.402 (9) | C96—C97 | 1.404 (9) |
| C49—C50 | 1.391 (9) | C98—H98A | 0.9800 |
| C49—H49 | 0.9500 | C98—H98B | 0.9800 |
| C50—C51 | 1.370 (12) | C98—H98C | 0.9800 |

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| O5—Sm1—O4 | 69.96 (17) | O3—C39—H39B | 109.5 |
| O5—Sm1—O9 | 119.1 (2) | H39A—C39—H39B | 109.5 |
| O4—Sm1—O9 | 116.53 (16) | O3—C39—H39C | 109.5 |
| O5—Sm1—O14 | 76.29 (18) | H39A—C39—H39C | 109.5 |
| O4—Sm1—O14 | 116.86 (16) | H39B—C39—H39C | 109.5 |
| O9—Sm1—O14 | 126.43 (17) | O3—C40—C41 | 127.1 (7) |
| O5—Sm1—O7 | 80.7 (2) | O3—C40—C45 | 111.9 (6) |
| O4—Sm1—O7 | 72.98 (17) | C41—C40—C45 | 121.0 (6) |
| O9—Sm1—O7 | 50.9 (2) | C40—C41—C42 | 120.7 (7) |
| O14—Sm1—O7 | 149.1 (3) | C40—C41—H41 | 119.7 |
| O5—Sm1—O11 | 143.01 (17) | C42—C41—H41 | 119.7 |
| O4—Sm1—O11 | 107.06 (18) | C41—C42—C43 | 119.4 (7) |
| O9—Sm1—O11 | 95.7 (2) | C41—C42—H42 | 120.3 |
| O14—Sm1—O11 | 72.73 (19) | C43—C42—H42 | 120.3 |
| O7—Sm1—O11 | 135.0 (2) | C42—C43—C44 | 120.9 (6) |
| O5—Sm1—O13 | 75.13 (18) | C42—C43—H43 | 119.6 |
| O4—Sm1—O13 | 69.89 (14) | C44—C43—H43 | 119.6 |
| O9—Sm1—O13 | 165.4 (2) | C46—C44—C43 | 119.5 (6) |
| O14—Sm1—O13 | 50.38 (17) | C46—C44—C45 | 120.1 (6) |
| O7—Sm1—O13 | 140.77 (17) | C43—C44—C45 | 120.0 (7) |
| O11—Sm1—O13 | 69.70 (17) | O4—C45—C44 | 122.4 (6) |
| O5—Sm1—O3 | 131.33 (15) | O4—C45—C40 | 119.7 (5) |

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| O4—Sm1—O3 | 62.37 (17) | C44—C45—C40 | 117.8 (6) |
| O9—Sm1—O3 | 76.7 (2) | N33—C46—C44 | 122.4 (6) |
| O14—Sm1—O3 | 134.1 (2) | N33—C46—H46 | 118.8 |
| O7—Sm1—O3 | 76.8 (2) | C44—C46—H46 | 118.8 |
| O11—Sm1—O3 | 65.28 (18) | N33—C47—C48 | 109.7 (5) |
| O13—Sm1—O3 | 96.56 (19) | N33—C47—C54 | 111.9 (4) |
| O5—Sm1—O6 | 63.17 (16) | C48—C47—C54 | 112.6 (5) |
| O4—Sm1—O6 | 129.40 (18) | N33—C47—H47 | 107.5 |
| O9—Sm1—O6 | 73.8 (2) | C48—C47—H47 | 107.5 |
| O14—Sm1—O6 | 69.72 (18) | C54—C47—H47 | 107.5 |
| O7—Sm1—O6 | 81.6 (2) | C49—C48—C53 | 119.3 (6) |
| O11—Sm1—O6 | 121.57 (16) | C49—C48—C47 | 121.8 (5) |
| O13—Sm1—O6 | 113.06 (17) | C53—C48—C47 | 118.9 (6) |
| O3—Sm1—O6 | 150.26 (17) | C50—C49—C48 | 120.1 (7) |
| O5—Sm1—O10 | 133.49 (17) | C50—C49—H49 | 120.0 |
| O4—Sm1—O10 | 154.62 (18) | C48—C49—H49 | 120.0 |
| O9—Sm1—O10 | 64.75 (18) | C51—C50—C49 | 120.0 (7) |
| O14—Sm1—O10 | 69.20 (18) | C51—C50—H50 | 120.0 |
| O7—Sm1—O10 | 115.43 (18) | C49—C50—H50 | 120.0 |
| O11—Sm1—O10 | 49.29 (17) | C50—C51—C52 | 120.8 (7) |
| O13—Sm1—O10 | 103.59 (16) | C50—C51—H51 | 119.6 |
| O3—Sm1—O10 | 95.18 (18) | C52—C51—H51 | 119.6 |
| O6—Sm1—O10 | 75.95 (17) | C52—C53—C48 | 120.0 (7) |
| O5—Sm1—N31 | 100.1 (2) | C52—C53—H53 | 120.0 |
| O4—Sm1—N31 | 95.06 (16) | C48—C53—H53 | 120.0 |
| O9—Sm1—N31 | 25.5 (2) | C53—C52—C51 | 119.8 (7) |
| O14—Sm1—N31 | 143.2 (2) | C53—C52—H52 | 120.1 |
| O7—Sm1—N31 | 25.4 (2) | C51—C52—H52 | 120.1 |
| O11—Sm1—N31 | 116.8 (2) | N32—C54—C55 | 110.7 (4) |
| O13—Sm1—N31 | 164.95 (16) | N32—C54—C47 | 110.3 (4) |
| O3—Sm1—N31 | 75.6 (2) | C55—C54—C47 | 115.2 (4) |
| O6—Sm1—N31 | 76.0 (2) | N32—C54—H54 | 106.7 |
| O10—Sm1—N31 | 90.08 (19) | C55—C54—H54 | 106.7 |
| O5—Sm1—N29 | 72.0 (2) | C47—C54—H54 | 106.7 |
| O4—Sm1—N29 | 92.41 (17) | C56—C55—C60 | 120.0 |
| O9—Sm1—N29 | 150.90 (17) | C56—C55—C54 | 118.8 (4) |
| O14—Sm1—N29 | 25.56 (18) | C60—C55—C54 | 121.2 (4) |
| O7—Sm1—N29 | 152.3 (2) | C55—C56—C57 | 120.0 |
| O11—Sm1—N29 | 71.3 (2) | C55—C56—H56 | 120.0 |
| O13—Sm1—N29 | 24.99 (18) | C57—C56—H56 | 120.0 |
| O3—Sm1—N29 | 117.7 (2) | C58—C57—C56 | 120.0 |
| O6—Sm1—N29 | 90.6 (2) | C58—C57—H57 | 120.0 |
| O10—Sm1—N29 | 87.92 (18) | C56—C57—H57 | 120.0 |
| N31—Sm1—N29 | 166.6 (3) | C59—C58—C57 | 120.0 |
| O18—Sm2—O17 | 69.48 (17) | C59—C58—H58 | 120.0 |
| O18—Sm2—O28 | 84.7 (2) | C57—C58—H58 | 120.0 |
| O17—Sm2—O28 | 71.80 (19) | C60—C59—C58 | 120.0 |
| O18—Sm2—O26 | 122.7 (2) | C60—C59—H59 | 120.0 |

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| O17—Sm2—O26 | 115.40 (15) | C58—C59—H59 | 120.0 |
| O28—Sm2—O26 | 50.61 (17) | C59—C60—C55 | 120.0 |
| O18—Sm2—O20 | 75.22 (19) | C59—C60—H60 | 120.0 |
| O17—Sm2—O20 | 118.48 (16) | C55—C60—H60 | 120.0 |
| O28—Sm2—O20 | 150.9 (3) | N32—C61—C62 | 121.5 (6) |
| O26—Sm2—O20 | 126.03 (15) | N32—C61—H61 | 119.2 |
| O18—Sm2—O24 | 139.72 (18) | C62—C61—H61 | 119.2 |
| O17—Sm2—O24 | 108.00 (18) | C67—C62—C61 | 121.4 (6) |
| O28—Sm2—O24 | 134.2 (2) | C67—C62—C63 | 119.3 (6) |
| O26—Sm2—O24 | 95.3 (2) | C61—C62—C63 | 119.2 (7) |
| O20—Sm2—O24 | 71.40 (19) | C64—C63—C62 | 120.3 (8) |
| O18—Sm2—O21 | 73.25 (19) | C64—C63—H63 | 119.9 |
| O17—Sm2—O21 | 71.42 (15) | C62—C63—H63 | 119.9 |
| O28—Sm2—O21 | 141.83 (17) | C63—C64—C65 | 120.3 (7) |
| O26—Sm2—O21 | 163.7 (2) | C63—C64—H64 | 119.9 |
| O20—Sm2—O21 | 50.65 (17) | C65—C64—H64 | 119.9 |
| O24—Sm2—O21 | 68.35 (18) | C66—C65—C64 | 122.0 (7) |
| O18—Sm2—O19 | 63.28 (17) | C66—C65—H65 | 119.0 |
| O17—Sm2—O19 | 126.05 (19) | C64—C65—H65 | 119.0 |
| O28—Sm2—O19 | 79.2 (2) | O6—C66—C65 | 127.5 (6) |
| O26—Sm2—O19 | 73.5 (2) | O6—C66—C67 | 113.4 (6) |
| O20—Sm2—O19 | 73.06 (19) | C65—C66—C67 | 119.2 (7) |
| O24—Sm2—O19 | 124.63 (16) | O5—C67—C62 | 122.6 (6) |
| O21—Sm2—O19 | 115.52 (19) | O5—C67—C66 | 118.4 (7) |
| O18—Sm2—O16 | 131.36 (15) | C62—C67—C66 | 119.0 (7) |
| O17—Sm2—O16 | 62.19 (17) | O6—C68—H68A | 109.5 |
| O28—Sm2—O16 | 75.9 (2) | O6—C68—H68B | 109.5 |
| O26—Sm2—O16 | 76.33 (19) | H68A—C68—H68B | 109.5 |
| O20—Sm2—O16 | 133.2 (2) | O6—C68—H68C | 109.5 |
| O24—Sm2—O16 | 65.47 (17) | H68A—C68—H68C | 109.5 |
| O21—Sm2—O16 | 95.62 (18) | H68B—C68—H68C | 109.5 |
| O19—Sm2—O16 | 148.86 (17) | O19—C69—H69A | 109.5 |
| O18—Sm2—O23 | 134.04 (16) | O19—C69—H69B | 109.5 |
| O17—Sm2—O23 | 154.52 (18) | H69A—C69—H69B | 109.5 |
| O28—Sm2—O23 | 114.47 (17) | O19—C69—H69C | 109.5 |
| O26—Sm2—O23 | 64.02 (15) | H69A—C69—H69C | 109.5 |
| O20—Sm2—O23 | 68.97 (16) | H69B—C69—H69C | 109.5 |
| O24—Sm2—O23 | 48.99 (15) | C71—C70—O19 | 125.9 (7) |
| O21—Sm2—O23 | 103.15 (15) | C71—C70—C75 | 122.1 (8) |
| O19—Sm2—O23 | 79.12 (16) | O19—C70—C75 | 112.0 (6) |
| O16—Sm2—O23 | 94.47 (15) | C70—C71—C72 | 119.6 (7) |
| O18—Sm2—N36 | 104.7 (2) | C70—C71—H71 | 120.2 |
| O17—Sm2—N36 | 93.42 (16) | C72—C71—H71 | 120.2 |
| O28—Sm2—N36 | 25.34 (18) | C73—C72—C71 | 120.5 (7) |
| O26—Sm2—N36 | 25.28 (15) | C73—C72—H72 | 119.7 |
| O20—Sm2—N36 | 144.42 (17) | C71—C72—H72 | 119.7 |
| O24—Sm2—N36 | 115.51 (18) | C72—C73—C74 | 120.0 (8) |
| O21—Sm2—N36 | 164.57 (15) | C72—C73—H73 | 120.0 |

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| O19—Sm2—N36 | 75.45 (19) | C74—C73—H73 | 120.0 |
| O16—Sm2—N36 | 74.01 (19) | C73—C74—C75 | 121.0 (6) |
| O23—Sm2—N36 | 89.26 (15) | C73—C74—C76 | 120.8 (6) |
| O18—Sm2—N34 | 71.2 (2) | C75—C74—C76 | 118.2 (6) |
| O17—Sm2—N34 | 94.85 (16) | O18—C75—C70 | 120.9 (7) |
| O28—Sm2—N34 | 155.5 (2) | O18—C75—C74 | 122.4 (6) |
| O26—Sm2—N34 | 149.31 (16) | C70—C75—C74 | 116.7 (7) |
| O20—Sm2—N34 | 25.05 (18) | N38—C76—C74 | 122.6 (6) |
| O24—Sm2—N34 | 68.9 (2) | N38—C76—H76 | 118.7 |
| O21—Sm2—N34 | 25.66 (18) | C74—C76—H76 | 118.7 |
| O19—Sm2—N34 | 93.5 (2) | N38—C77—C78 | 112.2 (4) |
| O16—Sm2—N34 | 116.7 (2) | N38—C77—C84 | 109.1 (4) |
| O23—Sm2—N34 | 86.55 (16) | C78—C77—C84 | 113.6 (5) |
| N36—Sm2—N34 | 168.7 (2) | N38—C77—H77 | 107.2 |
| C40—O3—C39 | 117.1 (6) | C78—C77—H77 | 107.2 |
| C40—O3—Sm1 | 116.5 (4) | C84—C77—H77 | 107.2 |
| C39—O3—Sm1 | 123.2 (4) | C79—C78—C83 | 118.8 (7) |
| C45—O4—Sm1 | 124.4 (4) | C79—C78—C77 | 118.0 (6) |
| C67—O5—Sm1 | 127.2 (4) | C83—C78—C77 | 123.1 (6) |
| C66—O6—C68 | 117.2 (6) | C78—C79—C80 | 121.5 (8) |
| C66—O6—Sm1 | 117.9 (4) | C78—C79—H79 | 119.2 |
| C68—O6—Sm1 | 124.9 (5) | C80—C79—H79 | 119.2 |
| N31—O7—Sm1 | 96.3 (5) | C81—C80—C79 | 119.8 (8) |
| N31—O9—Sm1 | 97.3 (4) | C81—C80—H80 | 120.1 |
| N30—O10—Sm1 | 94.0 (4) | C79—C80—H80 | 120.1 |
| N30—O11—Sm1 | 100.6 (5) | C80—C81—C82 | 118.6 (8) |
| N29—O13—Sm1 | 95.7 (4) | C80—C81—H81 | 120.7 |
| N29—O14—Sm1 | 97.9 (4) | C82—C81—H81 | 120.7 |
| C96—O16—C98 | 117.5 (7) | C83—C82—C81 | 121.0 (9) |
| C96—O16—Sm2 | 113.8 (4) | C83—C82—H82 | 128 (5) |
| C98—O16—Sm2 | 125.3 (4) | C81—C82—H82 | 110 (5) |
| C97—O17—Sm2 | 121.5 (4) | C82—C83—C78 | 120.2 (8) |
| C75—O18—Sm2 | 126.3 (4) | C82—C83—H83 | 119.9 |
| C70—O19—C69 | 116.4 (6) | C78—C83—H83 | 119.9 |
| C70—O19—Sm2 | 117.0 (4) | N37—C84—C85 | 113.1 (5) |
| C69—O19—Sm2 | 126.5 (5) | N37—C84—C77 | 108.5 (4) |
| N34—O20—Sm2 | 98.0 (4) | C85—C84—C77 | 109.8 (5) |
| N34—O21—Sm2 | 95.5 (4) | N37—C84—H84 | 108.4 |
| N35—O23—Sm2 | 95.2 (4) | C85—C84—H84 | 108.4 |
| N35—O24—Sm2 | 99.2 (4) | C77—C84—H84 | 108.4 |
| N36—O26—Sm2 | 96.8 (4) | C87—C86—C85 | 120.2 (6) |
| N36—O28—Sm2 | 97.6 (4) | C87—C86—H86 | 119.9 |
| O15—N29—O13 | 123.1 (8) | C85—C86—H86 | 119.9 |
| O15—N29—O14 | 121.5 (8) | C90—C85—C86 | 118.7 (6) |
| O13—N29—O14 | 115.3 (6) | C90—C85—C84 | 122.6 (6) |
| O15—N29—Sm1 | 174.1 (8) | C86—C85—C84 | 118.6 (5) |
| O13—N29—Sm1 | 59.3 (3) | C88—C87—C86 | 122.1 (8) |
| O14—N29—Sm1 | 56.6 (3) | C88—C87—H87 | 119.0 |

| | | | |
|---|---|---|---|
| O12—N30—O11 | 121.7 (7) | C86—C87—H87 | 119.0 |
| O12—N30—O10 | 122.2 (6) | C88—C89—C90 | 121.3 (8) |
| O11—N30—O10 | 116.1 (6) | C88—C89—H89 | 119.4 |
| O8—N31—O7 | 122.2 (8) | C90—C89—H89 | 119.4 |
| O8—N31—O9 | 122.3 (7) | C87—C88—C89 | 118.5 (7) |
| O7—N31—O9 | 115.5 (6) | C87—C88—H88 | 120.8 |
| O8—N31—Sm1 | 178.3 (7) | C89—C88—H88 | 120.8 |
| O7—N31—Sm1 | 58.3 (4) | C85—C90—C89 | 118.9 (8) |
| O9—N31—Sm1 | 57.2 (3) | C85—C90—H90 | 120.5 |
| C61—N32—C54 | 123.4 (5) | C89—C90—H90 | 120.5 |
| C61—N32—H32 | 114.0 | N37—C91—C92 | 122.8 (6) |
| C54—N32—H32 | 121.5 | N37—C91—H91 | 118.6 |
| C46—N33—C47 | 124.8 (5) | C92—C91—H91 | 118.6 |
| C46—N33—H33 | 119.8 | C97—C92—C93 | 119.3 (7) |
| C47—N33—H33 | 114.6 | C97—C92—C91 | 120.1 (6) |
| O22—N34—O20 | 122.0 (8) | C93—C92—C91 | 120.6 (6) |
| O22—N34—O21 | 122.3 (8) | C94—C93—C92 | 120.5 (7) |
| O20—N34—O21 | 115.7 (6) | C94—C93—H93 | 119.7 |
| O22—N34—Sm2 | 173.1 (8) | C92—C93—H93 | 119.7 |
| O20—N34—Sm2 | 57.0 (3) | C93—C94—C95 | 120.7 (7) |
| O21—N34—Sm2 | 58.9 (3) | C93—C94—H94 | 119.7 |
| O25—N35—O23 | 123.2 (5) | C95—C94—H94 | 119.7 |
| O25—N35—O24 | 120.2 (6) | C96—C95—C94 | 119.5 (7) |
| O23—N35—O24 | 116.6 (6) | C96—C95—H95 | 120.3 |
| O27—N36—O26 | 121.3 (6) | C94—C95—H95 | 120.3 |
| O27—N36—O28 | 123.8 (7) | C95—C96—O16 | 126.2 (7) |
| O26—N36—O28 | 114.9 (6) | C95—C96—C97 | 121.6 (6) |
| O27—N36—Sm2 | 178.5 (7) | O16—C96—C97 | 112.3 (6) |
| O26—N36—Sm2 | 57.9 (3) | O17—C97—C96 | 119.9 (6) |
| O28—N36—Sm2 | 57.0 (4) | O17—C97—C92 | 121.7 (6) |
| C91—N37—C84 | 125.5 (5) | C96—C97—C92 | 118.4 (6) |
| C91—N37—H37 | 107.3 | O16—C98—H98A | 109.5 |
| C84—N37—H37 | 122.8 | O16—C98—H98B | 109.5 |
| C76—N38—C77 | 125.8 (5) | H98A—C98—H98B | 109.5 |
| C76—N38—H38 | 119.5 | O16—C98—H98C | 109.5 |
| C77—N38—H38 | 114.7 | H98A—C98—H98C | 109.5 |
| O3—C39—H39A | 109.5 | H98B—C98—H98C | 109.5 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C98—H98*A*···O9$^{i}$ | 0.98 | 2.58 | 3.419 (9) | 144 |
| C91—H91···O27$^{ii}$ | 0.95 | 2.59 | 3.097 (8) | 114 |
| C91—H91···O12$^{iii}$ | 0.95 | 2.33 | 3.227 (8) | 156 |
| C77—H77···O24$^{iv}$ | 1.00 | 2.29 | 3.264 (8) | 164 |
| C76—H76···O21$^{iv}$ | 0.95 | 2.50 | 3.399 (9) | 158 |
| C69—H69*A*···O14$^{v}$ | 0.98 | 2.44 | 3.323 (10) | 150 |
| C68—H68*A*···O10 | 0.98 | 2.55 | 3.214 (11) | 125 |

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|---|---|---|---|---|
| C68—H68*A*···O9 | 0.98 | 2.66 | 3.224 (11) | 117 |
| C65—H65···O20$^{vi}$ | 0.95 | 2.64 | 3.485 (8) | 148 |
| C61—H61···O13$^{vi}$ | 0.95 | 2.49 | 3.429 (8) | 172 |
| C54—H54···O11$^{vi}$ | 1.00 | 2.30 | 3.277 (8) | 165 |
| C46—H46···O25 | 0.95 | 2.32 | 3.211 (8) | 155 |
| C46—H46···O8$^{i}$ | 0.95 | 2.56 | 3.054 (8) | 113 |
| C39—H39*A*···O27$^{i}$ | 0.98 | 2.54 | 3.338 (9) | 138 |
| N38—H38···O18 | 0.86 | 1.87 | 2.550 (6) | 135 |
| N33—H33···O4 | 0.86 | 1.87 | 2.545 (7) | 134 |
| N37—H37···O17 | 0.83 | 1.89 | 2.582 (7) | 139 |
| N32—H32···O5 | 1.04 | 1.71 | 2.578 (6) | 138 |

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