

Bis[μ -2-(4-hydroxyphenyl)acetato]- κ^3 O,O':O; κ^3 O:O,O'-bis[aqua(4,4'-bipyridine- κ N)][2-(4-hydroxyphenyl)acetato- κ^2 O,O']samarium(III) monohydrate

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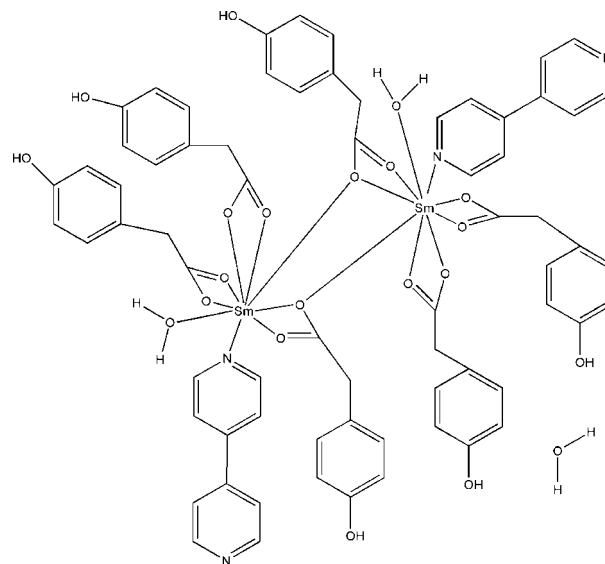
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.029; wR factor = 0.070; data-to-parameter ratio = 16.8.

The dinuclear title complex, $[\text{Sm}_2(\text{C}_8\text{H}_7\text{O}_3)_6(\text{C}_{10}\text{H}_8\text{N}_2)_2 \cdot (\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$, contains two Sm^{III} atoms, six deprotonated *p*-hydroxyphenylacetic acid (PAA) molecules, two 4,4'-bipyridine (bipy) molecules, two coordinated water molecules and one solvent water molecule. Each Sm^{III} ion is nine-coordinated by seven O atoms from four PAA ligands, one water O atom and one N atom from a bipy ligand in a distorted geometry. The PAA ligands are coordinated to the Sm^{III} ion in bridging and bridging tridentate modes. The asymmetric unit also contains one uncoordinated water molecule. The occurrence of numerous O—H...O and O—H...N hydrogen bonds involving coordinated and non-coordinated water molecules builds up an intricate three-dimensional network.

Related literature

For related structures, see: Arias *et al.* (2000); Liu *et al.* (2010). For applications of carboxylic metal-organic complexes, see: Wang & Sevov (2008); Wang *et al.* (2010); Fang & Zhang (2006).



Experimental

Crystal data

$[\text{Sm}_2(\text{C}_8\text{H}_7\text{O}_3)_6(\text{C}_{10}\text{H}_8\text{N}_2)_2 \cdot (\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$
 $M_r = 1573.96$
 Triclinic, $P\bar{1}$
 $a = 11.7589$ (3) Å
 $b = 16.3141$ (4) Å
 $c = 18.4618$ (5) Å
 $\alpha = 83.619$ (1)°

$\beta = 72.025$ (1)°
 $\gamma = 70.941$ (1)°
 $V = 3183.90$ (14) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.91$ mm⁻¹
 $T = 296$ K
 $0.34 \times 0.14 \times 0.03$ mm

Data collection

Bruker APEXII area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.733$, $T_{\text{max}} = 0.941$

49293 measured reflections
 14715 independent reflections
 11851 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.047$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.070$
 $S = 1.02$
 14715 reflections
 875 parameters
 9 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.66$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.72$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------|----------|-------------|-------------|---------------|
| O3—H3B...O12 ⁱ | 0.82 | 1.94 | 2.749 (3) | 169 |
| O6—H6B...O3W ⁱⁱ | 0.82 | 1.86 | 2.642 (3) | 159 |
| O9—H9A...O17 ⁱⁱⁱ | 0.82 | 1.86 | 2.673 (3) | 173 |
| O12—H12A...O11 ^{iv} | 0.82 | 1.94 | 2.746 (3) | 168 |
| O15—H15C...O6 ^v | 0.82 | 1.91 | 2.722 (3) | 174 |
| O18—H18B...O9 ⁱⁱ | 0.82 | 1.95 | 2.768 (3) | 173 |
| O2W—H2WA...O5 | 0.83 (5) | 2.02 (5) | 2.767 (3) | 150 (4) |
| O2W—H2WB...N2 ⁱⁱ | 0.83 (2) | 2.03 (2) | 2.841 (3) | 164 (5) |
| O3W—H3WB...O3 | 0.85 (4) | 1.99 (2) | 2.816 (3) | 167 (5) |
| O1W—H1WA...O13 | 0.81 (5) | 1.96 (4) | 2.755 (3) | 165 (4) |
| O1W—H1WB...N4 ⁱ | 0.83 (2) | 1.99 (2) | 2.778 (3) | 160 (4) |
| O3W—H3WA...O1 ^{vi} | 0.84 (4) | 1.94 (4) | 2.773 (3) | 172 (4) |

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

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2162).

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supplementary materials

Acta Cryst. (2010). E66, m1511-m1512 [doi:10.1107/S1600536810044454]

Bis[μ -2-(4-hydroxyphenyl)acetato]- $\kappa^3 O, O': O; \kappa^3 O: O, O'$ -bis{aqua(4,4'-bipyridine- κN)}]2-(4-hydroxyphenyl)acetato- $\kappa^2 O, O'$]samarium(III)} monohydrate

J.-L. Liu, J.-F. Liu and G.-L. Zhao

Comment

The design and synthesis of carboxylic metal-organic complexes have been an increasing interest for decades owing to their potential practical applications, such as fluorescence and magnetism (Wang, *et al.*, 2010; Fang *et al.*, 2006; Wang, *et al.*, 2008). We have published on this subject before (Liu, *et al.*, 2010). In the current paper we report the crystal structure of a new Sm^{III} complex with the ligand *p*-hydroxyphenylacetic acid. The title compound consist of six *L* ligands, two bipy molecules and two coordinated water molecules. In the dinuclear compound, each Sm ion is coordinated with seven O atoms from four *L* ligands, one N atom from 4,4'-bipyridine ligand and one O atom from a water molecule. The central Sm atom is nine coordinated. The PAA ligands are coordinating in two modes, bridging and bridging tridentate. (Fig.1). The Sm^{III} ion is in a distorted ball coordination geometry. The asymmetric unit further contains one solvent water molecule. Bond lengths and bond angles involving the metals and O atoms skeleton compare well with related structure as bis((μ 2-Acetato-*O, O, O'*)-diaqua-bis(acetato-*O, O'*)-samarium(iii))pentahydrate (Arias, *et al.*, 2000), In addition, numerous O—H \cdots O bonds involving both hydroxyl groups as well as coordinated and non-coordinated water molecules build up an intricate three-dimensional network (Table 1).

Experimental

All reagents and solvents used were of commercially available quality and were used without prior purification. *p*-hydroxyphenylacetic acid(HPAA) (0.456 g, 3 mmol) and sodium hydroxide (0.12 g, 3 mmol) were mixed together in water (10 ml). Sm(NO₃)₃ (0.336 g, 1 mmol), dissolved in water (10 ml), was added into the first solution. After stirring for an hour, an ethanol (5 ml) solution of 4,4'-bipyridine (0.156 g, 1 mmol) was slowly dripped into the mixture, followed by three hours stirring. After filtration, the filtrate was allowed to stand at room temperature and single crystals suitable for *X*-ray diffraction were obtained after a week.

Refinement

All H atoms attached to C atoms and *O*(hydroxyl) atom were fixed geometrically and treated as riding with C—H = 0.97 Å (methylene) or 0.93 Å (aromatic) and O—H = 0.82 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. H atoms of water molecule were located in a difference Fourier map and included in the subsequent refinement using restraints (O—H = 0.82 (1)Å and H \cdots H = 1.39 (2) Å) with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. In the last cycles of refinement they were treated as riding on their parent O atom.

Figures

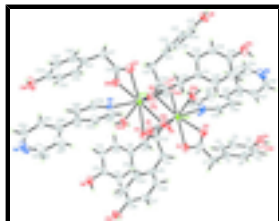


Fig. 1. The molecular structure of the title complex, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Bis[μ -2-(4-hydroxyphenyl)acetato]- $\kappa^3 O, O', O$; $\kappa^3 O:O, O'$ - bis{aqua(4,4'-bipyridine- κN)[2-(4-hydroxyphenyl)acetato- $\kappa^2 O, O'$]samarium(III)} monohydrate

Crystal data

[Sm₂(C₈H₇O₃)₆(C₁₀H₈N₂)₂(H₂O)₂]:H₂O

$M_r = 1573.96$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 11.7589$ (3) Å

$b = 16.3141$ (4) Å

$c = 18.4618$ (5) Å

$\alpha = 83.619$ (1)°

$\beta = 72.025$ (1)°

$\gamma = 70.941$ (1)°

$V = 3183.90$ (14) Å³

$Z = 2$

$F(000) = 1584$

$D_x = 1.642$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9956 reflections

$\theta = 1.7$ – 27.7 °

$\mu = 1.91$ mm⁻¹

$T = 296$ K

Block, colourless

$0.34 \times 0.14 \times 0.03$ mm

Data collection

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

phi and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.733$, $T_{\max} = 0.941$

49293 measured reflections

14715 independent reflections

11851 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\max} = 27.7$ °, $\theta_{\min} = 1.8$ °

$h = -15$ → 15

$k = -21$ → 21

$l = -24$ → 24

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.070$

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

| | |
|-------------------|--|
| $S = 1.02$ | $w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 0.993P]$ |
| 14715 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 875 parameters | $(\Delta/\sigma)_{\max} = 0.002$ |
| 9 restraints | $\Delta\rho_{\max} = 0.66 \text{ e } \text{\AA}^{-3}$ |
| | $\Delta\rho_{\min} = -0.72 \text{ e } \text{\AA}^{-3}$ |

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|---------------|--------------|----------------------------------|
| Sm1 | 0.271174 (13) | 0.364512 (8) | 0.283786 (7) | 0.02579 (4) |
| Sm2 | 0.131899 (13) | 0.206492 (8) | 0.195381 (7) | 0.02577 (4) |
| N1 | 0.3136 (2) | 0.51130 (14) | 0.28289 (14) | 0.0359 (6) |
| N2 | 0.3976 (3) | 0.92617 (19) | 0.2162 (2) | 0.0667 (10) |
| N3 | 0.0840 (2) | 0.06204 (14) | 0.18856 (13) | 0.0337 (5) |
| N4 | 0.0282 (4) | -0.36185 (19) | 0.2326 (2) | 0.0683 (10) |
| C1 | 0.2248 (3) | 0.51101 (19) | 0.51768 (16) | 0.0363 (7) |
| C2 | 0.3403 (3) | 0.5160 (2) | 0.47296 (17) | 0.0458 (8) |
| H2A | 0.3962 | 0.4689 | 0.4433 | 0.055* |
| C3 | 0.3750 (3) | 0.5896 (2) | 0.47116 (19) | 0.0505 (8) |
| H3A | 0.4533 | 0.5918 | 0.4404 | 0.061* |
| C4 | 0.2940 (3) | 0.6592 (2) | 0.51481 (19) | 0.0449 (8) |
| C5 | 0.1799 (3) | 0.6549 (2) | 0.56137 (19) | 0.0482 (8) |
| H5A | 0.1261 | 0.7013 | 0.5926 | 0.058* |
| C6 | 0.1449 (3) | 0.5823 (2) | 0.56210 (18) | 0.0445 (8) |
| H6A | 0.0664 | 0.5808 | 0.5929 | 0.053* |
| C7 | 0.1855 (3) | 0.4307 (2) | 0.52126 (16) | 0.0429 (8) |
| H7A | 0.2316 | 0.3855 | 0.5497 | 0.052* |
| H7B | 0.0967 | 0.4440 | 0.5481 | 0.052* |
| C8 | 0.2096 (3) | 0.39816 (19) | 0.44318 (16) | 0.0355 (7) |
| C9 | 0.6232 (3) | 0.08807 (18) | 0.30336 (18) | 0.0378 (7) |
| C10 | 0.6052 (3) | 0.0570 (2) | 0.37691 (18) | 0.0492 (8) |
| H10A | 0.5938 | 0.0937 | 0.4154 | 0.059* |
| C11 | 0.6033 (3) | -0.0276 (2) | 0.39568 (18) | 0.0494 (8) |
| H11A | 0.5911 | -0.0472 | 0.4459 | 0.059* |
| C12 | 0.6199 (3) | -0.08171 (18) | 0.33913 (17) | 0.0394 (7) |
| C13 | 0.6364 (3) | -0.0518 (2) | 0.26524 (17) | 0.0438 (8) |

supplementary materials

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|------|-------------|---------------|---------------|-------------|
| H13A | 0.6459 | -0.0882 | 0.2270 | 0.053* |
| C14 | 0.6389 (3) | 0.03153 (19) | 0.24766 (17) | 0.0432 (7) |
| H14A | 0.6515 | 0.0506 | 0.1973 | 0.052* |
| C15 | 0.6269 (3) | 0.17940 (19) | 0.2834 (2) | 0.0478 (8) |
| H15A | 0.6939 | 0.1783 | 0.2367 | 0.057* |
| H15B | 0.6475 | 0.2005 | 0.3233 | 0.057* |
| C16 | 0.5063 (3) | 0.24269 (17) | 0.27316 (16) | 0.0331 (6) |
| C17 | 0.2720 (3) | 0.4547 (2) | 0.01289 (16) | 0.0424 (8) |
| C18 | 0.1461 (4) | 0.5016 (2) | 0.02779 (17) | 0.0497 (9) |
| H18A | 0.0861 | 0.4747 | 0.0537 | 0.060* |
| C19 | 0.1070 (3) | 0.5873 (2) | 0.00524 (17) | 0.0453 (8) |
| H19A | 0.0218 | 0.6177 | 0.0158 | 0.054* |
| C20 | 0.1963 (3) | 0.62750 (19) | -0.03339 (17) | 0.0405 (7) |
| C21 | 0.3219 (3) | 0.58206 (19) | -0.04820 (17) | 0.0415 (7) |
| H21A | 0.3820 | 0.6090 | -0.0737 | 0.050* |
| C22 | 0.3589 (3) | 0.4964 (2) | -0.02525 (17) | 0.0434 (7) |
| H22A | 0.4442 | 0.4662 | -0.0357 | 0.052* |
| C23 | 0.3132 (4) | 0.3613 (2) | 0.03920 (17) | 0.0587 (10) |
| H23A | 0.2587 | 0.3316 | 0.0315 | 0.070* |
| H23B | 0.3981 | 0.3328 | 0.0085 | 0.070* |
| C24 | 0.3094 (3) | 0.35389 (17) | 0.12169 (15) | 0.0330 (6) |
| C25 | 0.1416 (3) | 0.11314 (19) | 0.47589 (16) | 0.0392 (7) |
| C26 | 0.0393 (3) | 0.1063 (2) | 0.53593 (17) | 0.0434 (7) |
| H26A | -0.0293 | 0.1554 | 0.5521 | 0.052* |
| C27 | 0.0378 (3) | 0.0273 (2) | 0.57213 (17) | 0.0421 (7) |
| H27A | -0.0312 | 0.0238 | 0.6125 | 0.051* |
| C28 | 0.1382 (3) | -0.04551 (19) | 0.54821 (16) | 0.0359 (7) |
| C29 | 0.2418 (3) | -0.0397 (2) | 0.48932 (17) | 0.0437 (7) |
| H29A | 0.3106 | -0.0888 | 0.4735 | 0.052* |
| C30 | 0.2428 (3) | 0.0393 (2) | 0.45411 (17) | 0.0436 (8) |
| H30A | 0.3131 | 0.0429 | 0.4148 | 0.052* |
| C31 | 0.1430 (4) | 0.1978 (2) | 0.43418 (17) | 0.0461 (8) |
| H31A | 0.2238 | 0.2058 | 0.4274 | 0.055* |
| H31B | 0.0791 | 0.2446 | 0.4657 | 0.055* |
| C32 | 0.1204 (3) | 0.20483 (17) | 0.35761 (15) | 0.0311 (6) |
| C33 | -0.2564 (3) | 0.48057 (17) | 0.24478 (16) | 0.0322 (6) |
| C34 | -0.2139 (3) | 0.51863 (19) | 0.17454 (17) | 0.0400 (7) |
| H34A | -0.1767 | 0.4845 | 0.1313 | 0.048* |
| C35 | -0.2258 (3) | 0.60528 (19) | 0.16781 (17) | 0.0412 (7) |
| H35A | -0.1963 | 0.6290 | 0.1203 | 0.049* |
| C36 | -0.2815 (3) | 0.65783 (18) | 0.23124 (17) | 0.0390 (7) |
| C37 | -0.3244 (3) | 0.62157 (19) | 0.30141 (17) | 0.0431 (7) |
| H37A | -0.3622 | 0.6560 | 0.3445 | 0.052* |
| C38 | -0.3109 (3) | 0.53371 (19) | 0.30752 (17) | 0.0396 (7) |
| H38A | -0.3394 | 0.5099 | 0.3552 | 0.048* |
| C39 | -0.2442 (3) | 0.38587 (17) | 0.25117 (18) | 0.0385 (7) |
| H39A | -0.2896 | 0.3738 | 0.3026 | 0.046* |
| H39B | -0.2848 | 0.3736 | 0.2171 | 0.046* |
| C40 | -0.1118 (3) | 0.32472 (17) | 0.23337 (15) | 0.0309 (6) |

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|------|-------------|---------------|---------------|-------------|
| C41 | 0.2359 (3) | 0.05195 (19) | -0.04822 (16) | 0.0395 (7) |
| C42 | 0.3536 (3) | 0.0011 (2) | -0.04455 (16) | 0.0430 (7) |
| H42A | 0.4101 | 0.0278 | -0.0405 | 0.052* |
| C43 | 0.3896 (3) | -0.0878 (2) | -0.04677 (17) | 0.0458 (8) |
| H43A | 0.4701 | -0.1206 | -0.0452 | 0.055* |
| C44 | 0.3057 (3) | -0.1283 (2) | -0.05126 (18) | 0.0483 (8) |
| C45 | 0.1879 (3) | -0.0793 (2) | -0.05580 (19) | 0.0506 (8) |
| H45A | 0.1316 | -0.1062 | -0.0598 | 0.061* |
| C46 | 0.1538 (3) | 0.0102 (2) | -0.05431 (17) | 0.0466 (8) |
| H46A | 0.0742 | 0.0431 | -0.0575 | 0.056* |
| C47 | 0.1936 (3) | 0.1500 (2) | -0.04211 (17) | 0.0464 (8) |
| H47A | 0.2564 | 0.1724 | -0.0781 | 0.056* |
| H47B | 0.1156 | 0.1742 | -0.0556 | 0.056* |
| C48 | 0.1739 (3) | 0.17845 (18) | 0.03700 (16) | 0.0358 (7) |
| C49 | 0.2317 (3) | 0.58065 (18) | 0.32245 (17) | 0.0385 (7) |
| H49A | 0.1590 | 0.5745 | 0.3578 | 0.046* |
| C50 | 0.2495 (3) | 0.66107 (18) | 0.31352 (17) | 0.0404 (7) |
| H50A | 0.1897 | 0.7075 | 0.3426 | 0.048* |
| C51 | 0.3563 (3) | 0.67260 (18) | 0.26136 (17) | 0.0377 (7) |
| C52 | 0.4429 (3) | 0.60032 (19) | 0.22209 (19) | 0.0455 (8) |
| H52A | 0.5175 | 0.6044 | 0.1874 | 0.055* |
| C53 | 0.4187 (3) | 0.52211 (19) | 0.23437 (19) | 0.0435 (8) |
| H53A | 0.4787 | 0.4742 | 0.2074 | 0.052* |
| C54 | 0.4496 (4) | 0.8649 (2) | 0.1638 (3) | 0.0724 (13) |
| H54A | 0.4949 | 0.8787 | 0.1158 | 0.087* |
| C55 | 0.4407 (3) | 0.7819 (2) | 0.1761 (2) | 0.0588 (10) |
| H55A | 0.4788 | 0.7417 | 0.1371 | 0.071* |
| C56 | 0.3751 (3) | 0.75940 (19) | 0.24675 (19) | 0.0427 (8) |
| C57 | 0.3238 (4) | 0.8221 (2) | 0.3018 (2) | 0.0613 (10) |
| H57A | 0.2810 | 0.8096 | 0.3511 | 0.074* |
| C58 | 0.3363 (5) | 0.9036 (2) | 0.2835 (3) | 0.0726 (12) |
| H58A | 0.2988 | 0.9452 | 0.3214 | 0.087* |
| C59 | 0.1697 (3) | -0.00447 (18) | 0.14641 (17) | 0.0406 (7) |
| H59A | 0.2428 | 0.0042 | 0.1136 | 0.049* |
| C60 | 0.1549 (3) | -0.08558 (18) | 0.14936 (17) | 0.0420 (7) |
| H60A | 0.2165 | -0.1294 | 0.1180 | 0.050* |
| C61 | 0.0493 (3) | -0.10176 (18) | 0.19860 (17) | 0.0376 (7) |
| C62 | -0.0413 (3) | -0.03205 (19) | 0.24020 (18) | 0.0417 (7) |
| H62A | -0.1156 | -0.0390 | 0.2729 | 0.050* |
| C63 | -0.0217 (3) | 0.04762 (18) | 0.23331 (17) | 0.0390 (7) |
| H63A | -0.0850 | 0.0936 | 0.2611 | 0.047* |
| C64 | 0.1071 (5) | -0.3394 (2) | 0.1717 (2) | 0.0729 (13) |
| H64A | 0.1613 | -0.3824 | 0.1370 | 0.088* |
| C65 | 0.1141 (4) | -0.2559 (2) | 0.1565 (2) | 0.0635 (11) |
| H65A | 0.1694 | -0.2436 | 0.1116 | 0.076* |
| C66 | 0.0382 (3) | -0.19087 (19) | 0.20833 (19) | 0.0445 (8) |
| C67 | -0.0452 (3) | -0.2136 (2) | 0.2724 (2) | 0.0622 (11) |
| H67A | -0.0988 | -0.1725 | 0.3090 | 0.075* |
| C68 | -0.0474 (4) | -0.2986 (2) | 0.2811 (3) | 0.0751 (14) |

supplementary materials

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|------|---------------|---------------|---------------|-------------|
| H68A | -0.1056 | -0.3124 | 0.3236 | 0.090* |
| O1W | 0.0812 (2) | 0.45996 (13) | 0.25489 (13) | 0.0402 (5) |
| O1 | 0.3063 (2) | 0.33572 (14) | 0.41483 (12) | 0.0464 (5) |
| O2W | 0.3290 (2) | 0.11013 (13) | 0.21451 (13) | 0.0413 (5) |
| O2 | 0.13551 (19) | 0.43506 (13) | 0.40444 (11) | 0.0393 (5) |
| O3 | 0.3309 (2) | 0.73187 (16) | 0.51131 (16) | 0.0669 (7) |
| H3B | 0.2729 | 0.7703 | 0.5372 | 0.057 (12)* |
| O3W | 0.5581 (3) | 0.76686 (17) | 0.49096 (15) | 0.0579 (6) |
| O4 | 0.49742 (19) | 0.32158 (12) | 0.26433 (13) | 0.0470 (6) |
| O5 | 0.41478 (19) | 0.21718 (12) | 0.27608 (12) | 0.0400 (5) |
| O6 | 0.6210 (3) | -0.16638 (13) | 0.35286 (12) | 0.0596 (7) |
| H6B | 0.5940 | -0.1742 | 0.3988 | 0.089* |
| O7 | 0.3524 (2) | 0.40008 (14) | 0.14780 (11) | 0.0460 (6) |
| O8 | 0.25816 (18) | 0.30140 (11) | 0.16494 (10) | 0.0319 (4) |
| O9 | 0.1635 (2) | 0.71240 (14) | -0.05719 (14) | 0.0560 (6) |
| H9A | 0.0928 | 0.7265 | -0.0624 | 0.084* |
| O10 | 0.14230 (18) | 0.26764 (11) | 0.31403 (10) | 0.0308 (4) |
| O11 | 0.0819 (2) | 0.15184 (12) | 0.33561 (10) | 0.0379 (5) |
| O12 | 0.1417 (2) | -0.12554 (13) | 0.58163 (12) | 0.0468 (5) |
| H12A | 0.0699 | -0.1259 | 0.6043 | 0.070* |
| O13 | -0.01795 (18) | 0.35213 (12) | 0.20644 (12) | 0.0396 (5) |
| O14 | -0.09509 (19) | 0.24475 (12) | 0.24404 (12) | 0.0436 (5) |
| O15 | -0.2918 (2) | 0.74357 (13) | 0.22099 (13) | 0.0563 (6) |
| H15C | -0.3183 | 0.7671 | 0.2626 | 0.084* |
| O16 | 0.2617 (2) | 0.15313 (13) | 0.06689 (11) | 0.0410 (5) |
| O17 | 0.0674 (2) | 0.22729 (14) | 0.07417 (12) | 0.0479 (5) |
| O18 | 0.3448 (3) | -0.21694 (15) | -0.05145 (16) | 0.0742 (8) |
| H18B | 0.2885 | -0.2341 | -0.0549 | 0.111* |
| H2WA | 0.377 (4) | 0.125 (3) | 0.231 (3) | 0.111* |
| H2WB | 0.362 (4) | 0.0568 (13) | 0.208 (3) | 0.111* |
| H3WB | 0.497 (3) | 0.748 (3) | 0.495 (3) | 0.111* |
| H1WA | 0.043 (4) | 0.436 (2) | 0.239 (3) | 0.111* |
| H1WB | 0.048 (4) | 0.5124 (12) | 0.249 (3) | 0.111* |
| H3WA | 0.594 (4) | 0.734 (3) | 0.521 (2) | 0.111* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Sm1 | 0.02854 (8) | 0.01798 (7) | 0.03435 (8) | -0.00970 (6) | -0.01220 (6) | 0.00222 (5) |
| Sm2 | 0.02720 (8) | 0.01720 (7) | 0.03501 (8) | -0.00788 (6) | -0.01100 (6) | 0.00011 (5) |
| N1 | 0.0358 (15) | 0.0245 (12) | 0.0504 (15) | -0.0115 (11) | -0.0146 (12) | -0.0006 (10) |
| N2 | 0.065 (2) | 0.0320 (16) | 0.121 (3) | -0.0237 (16) | -0.049 (2) | 0.0175 (18) |
| N3 | 0.0388 (15) | 0.0216 (11) | 0.0433 (14) | -0.0100 (10) | -0.0154 (11) | 0.0014 (10) |
| N4 | 0.084 (3) | 0.0323 (17) | 0.119 (3) | -0.0256 (17) | -0.070 (2) | 0.0171 (18) |
| C1 | 0.0403 (18) | 0.0384 (16) | 0.0334 (15) | -0.0138 (14) | -0.0124 (13) | -0.0034 (12) |
| C2 | 0.0385 (19) | 0.0460 (19) | 0.0467 (18) | -0.0089 (15) | -0.0036 (15) | -0.0133 (14) |
| C3 | 0.0343 (18) | 0.053 (2) | 0.060 (2) | -0.0180 (16) | 0.0001 (16) | -0.0114 (16) |
| C4 | 0.0403 (19) | 0.0419 (18) | 0.055 (2) | -0.0162 (15) | -0.0129 (16) | -0.0037 (14) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C5 | 0.0385 (19) | 0.0425 (18) | 0.059 (2) | -0.0096 (15) | -0.0063 (16) | -0.0140 (15) |
| C6 | 0.0358 (18) | 0.0426 (18) | 0.0514 (19) | -0.0124 (15) | -0.0034 (15) | -0.0115 (14) |
| C7 | 0.056 (2) | 0.0414 (18) | 0.0351 (16) | -0.0220 (16) | -0.0108 (15) | 0.0002 (13) |
| C8 | 0.0425 (19) | 0.0340 (16) | 0.0354 (15) | -0.0216 (14) | -0.0093 (14) | 0.0027 (12) |
| C9 | 0.0284 (16) | 0.0280 (15) | 0.060 (2) | -0.0047 (12) | -0.0215 (14) | -0.0002 (13) |
| C10 | 0.067 (2) | 0.0310 (17) | 0.0507 (19) | -0.0045 (16) | -0.0273 (18) | -0.0096 (14) |
| C11 | 0.069 (2) | 0.0375 (18) | 0.0395 (17) | -0.0109 (16) | -0.0179 (17) | -0.0032 (13) |
| C12 | 0.0428 (19) | 0.0300 (15) | 0.0434 (17) | -0.0105 (13) | -0.0105 (14) | -0.0006 (12) |
| C13 | 0.056 (2) | 0.0346 (17) | 0.0419 (17) | -0.0125 (15) | -0.0155 (15) | -0.0059 (13) |
| C14 | 0.051 (2) | 0.0368 (17) | 0.0403 (17) | -0.0120 (15) | -0.0145 (15) | 0.0047 (13) |
| C15 | 0.0329 (18) | 0.0280 (16) | 0.088 (2) | -0.0069 (13) | -0.0296 (17) | 0.0056 (15) |
| C16 | 0.0306 (16) | 0.0269 (14) | 0.0416 (16) | -0.0067 (12) | -0.0124 (13) | -0.0004 (11) |
| C17 | 0.066 (2) | 0.0394 (17) | 0.0331 (16) | -0.0272 (17) | -0.0205 (15) | 0.0043 (12) |
| C18 | 0.067 (3) | 0.063 (2) | 0.0339 (16) | -0.045 (2) | -0.0108 (16) | 0.0033 (15) |
| C19 | 0.0409 (19) | 0.056 (2) | 0.0424 (18) | -0.0187 (16) | -0.0106 (15) | -0.0078 (15) |
| C20 | 0.053 (2) | 0.0359 (16) | 0.0438 (17) | -0.0191 (15) | -0.0251 (15) | 0.0029 (13) |
| C21 | 0.046 (2) | 0.0366 (17) | 0.0500 (18) | -0.0219 (15) | -0.0177 (15) | 0.0086 (13) |
| C22 | 0.051 (2) | 0.0382 (17) | 0.0470 (18) | -0.0170 (15) | -0.0214 (16) | 0.0045 (13) |
| C23 | 0.112 (3) | 0.0389 (18) | 0.0380 (18) | -0.037 (2) | -0.0281 (19) | 0.0078 (14) |
| C24 | 0.0423 (18) | 0.0254 (14) | 0.0322 (14) | -0.0139 (13) | -0.0086 (13) | 0.0006 (11) |
| C25 | 0.058 (2) | 0.0380 (17) | 0.0354 (16) | -0.0256 (16) | -0.0236 (15) | 0.0076 (12) |
| C26 | 0.052 (2) | 0.0332 (16) | 0.0448 (18) | -0.0104 (15) | -0.0177 (16) | -0.0001 (13) |
| C27 | 0.0437 (19) | 0.0457 (18) | 0.0366 (16) | -0.0181 (15) | -0.0084 (14) | 0.0049 (13) |
| C28 | 0.0446 (19) | 0.0354 (16) | 0.0358 (15) | -0.0204 (14) | -0.0179 (14) | 0.0096 (12) |
| C29 | 0.043 (2) | 0.0442 (18) | 0.0441 (18) | -0.0155 (15) | -0.0135 (15) | 0.0063 (14) |
| C30 | 0.047 (2) | 0.051 (2) | 0.0387 (17) | -0.0268 (17) | -0.0119 (15) | 0.0109 (14) |
| C31 | 0.072 (2) | 0.0375 (17) | 0.0451 (18) | -0.0312 (17) | -0.0274 (17) | 0.0092 (13) |
| C32 | 0.0301 (16) | 0.0266 (14) | 0.0387 (15) | -0.0133 (12) | -0.0089 (12) | 0.0021 (11) |
| C33 | 0.0274 (15) | 0.0256 (14) | 0.0424 (16) | -0.0039 (11) | -0.0123 (13) | -0.0026 (11) |
| C34 | 0.0435 (19) | 0.0350 (16) | 0.0377 (16) | -0.0063 (14) | -0.0088 (14) | -0.0122 (12) |
| C35 | 0.047 (2) | 0.0363 (17) | 0.0385 (16) | -0.0137 (14) | -0.0100 (14) | 0.0015 (13) |
| C36 | 0.0421 (19) | 0.0273 (15) | 0.0491 (18) | -0.0069 (13) | -0.0192 (15) | -0.0014 (12) |
| C37 | 0.052 (2) | 0.0341 (16) | 0.0404 (17) | -0.0069 (15) | -0.0140 (15) | -0.0077 (13) |
| C38 | 0.0403 (18) | 0.0344 (16) | 0.0390 (16) | -0.0077 (13) | -0.0087 (14) | 0.0001 (12) |
| C39 | 0.0309 (17) | 0.0268 (15) | 0.0569 (19) | -0.0050 (12) | -0.0144 (14) | -0.0035 (13) |
| C40 | 0.0306 (16) | 0.0234 (13) | 0.0403 (15) | -0.0060 (12) | -0.0138 (13) | -0.0036 (11) |
| C41 | 0.050 (2) | 0.0382 (17) | 0.0303 (15) | -0.0157 (15) | -0.0087 (14) | -0.0027 (12) |
| C42 | 0.048 (2) | 0.0441 (18) | 0.0407 (17) | -0.0219 (16) | -0.0106 (15) | -0.0005 (13) |
| C43 | 0.048 (2) | 0.0385 (18) | 0.0484 (19) | -0.0121 (15) | -0.0103 (15) | -0.0027 (14) |
| C44 | 0.059 (2) | 0.0353 (17) | 0.0499 (19) | -0.0194 (16) | -0.0095 (17) | -0.0024 (14) |
| C45 | 0.053 (2) | 0.049 (2) | 0.057 (2) | -0.0267 (18) | -0.0118 (17) | -0.0055 (16) |
| C46 | 0.043 (2) | 0.049 (2) | 0.0451 (18) | -0.0098 (16) | -0.0112 (15) | -0.0086 (14) |
| C47 | 0.062 (2) | 0.0369 (17) | 0.0376 (17) | -0.0106 (16) | -0.0155 (16) | 0.0003 (13) |
| C48 | 0.050 (2) | 0.0246 (14) | 0.0339 (15) | -0.0152 (14) | -0.0098 (14) | 0.0010 (11) |
| C49 | 0.0425 (19) | 0.0296 (15) | 0.0442 (17) | -0.0142 (14) | -0.0111 (14) | 0.0019 (12) |
| C50 | 0.0465 (19) | 0.0244 (15) | 0.0516 (18) | -0.0103 (13) | -0.0165 (15) | -0.0014 (12) |
| C51 | 0.0402 (18) | 0.0245 (14) | 0.0552 (18) | -0.0129 (13) | -0.0222 (15) | 0.0044 (12) |
| C52 | 0.0345 (18) | 0.0329 (16) | 0.070 (2) | -0.0153 (14) | -0.0117 (16) | 0.0025 (15) |
| C53 | 0.0365 (18) | 0.0257 (15) | 0.067 (2) | -0.0103 (13) | -0.0112 (16) | -0.0048 (14) |

supplementary materials

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|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C54 | 0.054 (3) | 0.041 (2) | 0.114 (3) | -0.0220 (19) | -0.013 (2) | 0.023 (2) |
| C55 | 0.049 (2) | 0.0320 (18) | 0.085 (3) | -0.0160 (16) | -0.0029 (19) | 0.0024 (17) |
| C56 | 0.0408 (19) | 0.0270 (15) | 0.069 (2) | -0.0149 (14) | -0.0258 (16) | 0.0054 (14) |
| C57 | 0.094 (3) | 0.0378 (19) | 0.065 (2) | -0.031 (2) | -0.033 (2) | 0.0052 (16) |
| C58 | 0.112 (4) | 0.039 (2) | 0.089 (3) | -0.034 (2) | -0.049 (3) | 0.0000 (19) |
| C59 | 0.0458 (19) | 0.0291 (15) | 0.0432 (17) | -0.0120 (14) | -0.0086 (15) | 0.0028 (12) |
| C60 | 0.051 (2) | 0.0242 (15) | 0.0479 (18) | -0.0088 (14) | -0.0123 (15) | -0.0038 (12) |
| C61 | 0.0477 (19) | 0.0276 (15) | 0.0493 (17) | -0.0142 (14) | -0.0303 (15) | 0.0072 (12) |
| C62 | 0.0391 (18) | 0.0327 (16) | 0.0574 (19) | -0.0172 (14) | -0.0145 (15) | 0.0034 (14) |
| C63 | 0.0381 (18) | 0.0269 (15) | 0.0547 (18) | -0.0122 (13) | -0.0145 (15) | -0.0014 (13) |
| C64 | 0.133 (4) | 0.035 (2) | 0.076 (3) | -0.028 (2) | -0.063 (3) | -0.0010 (18) |
| C65 | 0.118 (4) | 0.0349 (19) | 0.055 (2) | -0.032 (2) | -0.043 (2) | 0.0041 (15) |
| C66 | 0.056 (2) | 0.0276 (15) | 0.066 (2) | -0.0162 (15) | -0.0398 (18) | 0.0080 (14) |
| C67 | 0.045 (2) | 0.0343 (18) | 0.109 (3) | -0.0162 (16) | -0.026 (2) | 0.0130 (19) |
| C68 | 0.054 (3) | 0.039 (2) | 0.145 (4) | -0.0274 (19) | -0.044 (3) | 0.030 (2) |
| O1W | 0.0430 (13) | 0.0232 (10) | 0.0624 (14) | -0.0089 (9) | -0.0288 (11) | 0.0028 (9) |
| O1 | 0.0521 (15) | 0.0388 (12) | 0.0462 (12) | -0.0040 (11) | -0.0207 (11) | -0.0047 (10) |
| O2W | 0.0404 (13) | 0.0237 (10) | 0.0655 (14) | -0.0073 (9) | -0.0257 (11) | -0.0013 (10) |
| O2 | 0.0383 (12) | 0.0408 (12) | 0.0412 (11) | -0.0132 (10) | -0.0135 (10) | -0.0021 (9) |
| O3 | 0.0475 (15) | 0.0463 (14) | 0.105 (2) | -0.0237 (13) | -0.0038 (15) | -0.0185 (14) |
| O3W | 0.0609 (18) | 0.0564 (16) | 0.0613 (16) | -0.0235 (14) | -0.0260 (13) | 0.0190 (12) |
| O4 | 0.0360 (12) | 0.0236 (10) | 0.0820 (16) | -0.0104 (9) | -0.0201 (11) | 0.0091 (10) |
| O5 | 0.0338 (12) | 0.0249 (10) | 0.0686 (14) | -0.0079 (9) | -0.0251 (10) | -0.0035 (9) |
| O6 | 0.096 (2) | 0.0339 (12) | 0.0485 (13) | -0.0285 (13) | -0.0118 (13) | -0.0006 (10) |
| O7 | 0.0632 (15) | 0.0504 (13) | 0.0399 (12) | -0.0408 (12) | -0.0145 (11) | 0.0078 (9) |
| O8 | 0.0365 (11) | 0.0243 (10) | 0.0378 (10) | -0.0148 (8) | -0.0106 (9) | 0.0039 (8) |
| O9 | 0.0606 (16) | 0.0360 (12) | 0.0839 (17) | -0.0159 (11) | -0.0408 (14) | 0.0096 (11) |
| O10 | 0.0356 (11) | 0.0241 (9) | 0.0349 (10) | -0.0144 (8) | -0.0096 (8) | 0.0049 (7) |
| O11 | 0.0527 (14) | 0.0350 (11) | 0.0373 (11) | -0.0272 (10) | -0.0170 (10) | 0.0073 (8) |
| O12 | 0.0511 (14) | 0.0344 (11) | 0.0541 (13) | -0.0201 (10) | -0.0117 (11) | 0.0130 (9) |
| O13 | 0.0279 (11) | 0.0236 (10) | 0.0687 (14) | -0.0064 (8) | -0.0167 (10) | -0.0029 (9) |
| O14 | 0.0330 (12) | 0.0220 (10) | 0.0713 (15) | -0.0078 (9) | -0.0105 (10) | 0.0022 (9) |
| O15 | 0.0844 (19) | 0.0294 (12) | 0.0591 (14) | -0.0195 (12) | -0.0253 (13) | 0.0020 (10) |
| O16 | 0.0394 (13) | 0.0397 (12) | 0.0450 (12) | -0.0109 (10) | -0.0131 (10) | -0.0062 (9) |
| O17 | 0.0487 (14) | 0.0455 (13) | 0.0436 (12) | 0.0021 (11) | -0.0204 (11) | -0.0075 (10) |
| O18 | 0.077 (2) | 0.0375 (14) | 0.112 (2) | -0.0190 (14) | -0.0312 (17) | -0.0027 (14) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|----------|-----------|
| Sm1—O5 | 2.4344 (19) | C28—O12 | 1.374 (3) |
| Sm1—O4 | 2.439 (2) | C28—C29 | 1.382 (4) |
| Sm1—O1W | 2.445 (2) | C29—C30 | 1.379 (4) |
| Sm1—O10 | 2.4396 (16) | C29—H29A | 0.9300 |
| Sm1—O2 | 2.451 (2) | C30—H30A | 0.9300 |
| Sm1—O7 | 2.4718 (19) | C31—C32 | 1.502 (4) |
| Sm1—O1 | 2.546 (2) | C31—H31A | 0.9700 |
| Sm1—O8 | 2.5904 (18) | C31—H31B | 0.9700 |
| Sm1—N1 | 2.598 (2) | C32—O11 | 1.251 (3) |
| Sm1—C16 | 2.792 (3) | C32—O10 | 1.274 (3) |

| | | | |
|----------|-------------|----------|-----------|
| Sm1—C8 | 2.876 (3) | C33—C38 | 1.381 (4) |
| Sm1—C24 | 2.902 (3) | C33—C34 | 1.393 (4) |
| Sm2—O8 | 2.3896 (16) | C33—C39 | 1.499 (4) |
| Sm2—O14 | 2.424 (2) | C34—C35 | 1.370 (4) |
| Sm2—O13 | 2.4379 (19) | C34—H34A | 0.9300 |
| Sm2—O2W | 2.444 (2) | C35—C36 | 1.385 (4) |
| Sm2—O16 | 2.464 (2) | C35—H35A | 0.9300 |
| Sm2—O17 | 2.532 (2) | C36—O15 | 1.361 (3) |
| Sm2—O10 | 2.5572 (18) | C36—C37 | 1.380 (4) |
| Sm2—O11 | 2.5947 (18) | C37—C38 | 1.385 (4) |
| Sm2—N3 | 2.620 (2) | C37—H37A | 0.9300 |
| Sm2—C40 | 2.806 (3) | C38—H38A | 0.9300 |
| Sm2—C48 | 2.874 (3) | C39—C40 | 1.506 (4) |
| Sm2—C32 | 2.954 (3) | C39—H39A | 0.9700 |
| N1—C53 | 1.336 (4) | C39—H39B | 0.9700 |
| N1—C49 | 1.334 (4) | C40—O14 | 1.257 (3) |
| N2—C58 | 1.312 (5) | C40—O13 | 1.265 (3) |
| N2—C54 | 1.326 (5) | C41—C42 | 1.380 (4) |
| N3—C63 | 1.341 (4) | C41—C46 | 1.386 (4) |
| N3—C59 | 1.337 (4) | C41—C47 | 1.517 (4) |
| N4—C64 | 1.320 (5) | C42—C43 | 1.373 (4) |
| N4—C68 | 1.331 (6) | C42—H42A | 0.9300 |
| C1—C2 | 1.378 (4) | C43—C44 | 1.380 (4) |
| C1—C6 | 1.389 (4) | C43—H43A | 0.9300 |
| C1—C7 | 1.514 (4) | C44—O18 | 1.368 (4) |
| C2—C3 | 1.383 (4) | C44—C45 | 1.378 (5) |
| C2—H2A | 0.9300 | C45—C46 | 1.383 (4) |
| C3—C4 | 1.367 (4) | C45—H45A | 0.9300 |
| C3—H3A | 0.9300 | C46—H46A | 0.9300 |
| C4—C5 | 1.372 (4) | C47—C48 | 1.508 (4) |
| C4—O3 | 1.378 (4) | C47—H47A | 0.9700 |
| C5—C6 | 1.372 (4) | C47—H47B | 0.9700 |
| C5—H5A | 0.9300 | C48—O16 | 1.250 (4) |
| C6—H6A | 0.9300 | C48—O17 | 1.271 (4) |
| C7—C8 | 1.503 (4) | C49—C50 | 1.379 (4) |
| C7—H7A | 0.9700 | C49—H49A | 0.9300 |
| C7—H7B | 0.9700 | C50—C51 | 1.381 (4) |
| C8—O1 | 1.264 (4) | C50—H50A | 0.9300 |
| C8—O2 | 1.257 (4) | C51—C52 | 1.380 (4) |
| C9—C10 | 1.373 (4) | C51—C56 | 1.486 (4) |
| C9—C14 | 1.387 (4) | C52—C53 | 1.376 (4) |
| C9—C15 | 1.506 (4) | C52—H52A | 0.9300 |
| C10—C11 | 1.392 (4) | C53—H53A | 0.9300 |
| C10—H10A | 0.9300 | C54—C55 | 1.380 (4) |
| C11—C12 | 1.369 (4) | C54—H54A | 0.9300 |
| C11—H11A | 0.9300 | C55—C56 | 1.374 (5) |
| C12—C13 | 1.374 (4) | C55—H55A | 0.9300 |
| C12—O6 | 1.373 (3) | C56—C57 | 1.376 (5) |
| C13—C14 | 1.369 (4) | C57—C58 | 1.378 (5) |

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| C13—H13A | 0.9300 | C57—H57A | 0.9300 |
| C14—H14A | 0.9300 | C58—H58A | 0.9300 |
| C15—C16 | 1.509 (4) | C59—C60 | 1.383 (4) |
| C15—H15A | 0.9700 | C59—H59A | 0.9300 |
| C15—H15B | 0.9700 | C60—C61 | 1.380 (4) |
| C16—O4 | 1.253 (3) | C60—H60A | 0.9300 |
| C16—O5 | 1.260 (3) | C61—C62 | 1.384 (4) |
| C17—C22 | 1.381 (4) | C61—C66 | 1.488 (4) |
| C17—C18 | 1.381 (5) | C62—C63 | 1.378 (4) |
| C17—C23 | 1.514 (4) | C62—H62A | 0.9300 |
| C18—C19 | 1.382 (5) | C63—H63A | 0.9300 |
| C18—H18A | 0.9300 | C64—C65 | 1.384 (5) |
| C19—C20 | 1.387 (4) | C64—H64A | 0.9300 |
| C19—H19A | 0.9300 | C65—C66 | 1.385 (5) |
| C20—O9 | 1.372 (3) | C65—H65A | 0.9300 |
| C20—C21 | 1.373 (4) | C66—C67 | 1.388 (5) |
| C21—C22 | 1.381 (4) | C67—C68 | 1.385 (5) |
| C21—H21A | 0.9300 | C67—H67A | 0.9300 |
| C22—H22A | 0.9300 | C68—H68A | 0.9300 |
| C23—C24 | 1.502 (4) | O1W—H1WA | 0.81 (5) |
| C23—H23A | 0.9700 | O1W—H1WB | 0.826 (18) |
| C23—H23B | 0.9700 | O2W—H2WA | 0.83 (5) |
| C24—O7 | 1.239 (3) | O2W—H2WB | 0.834 (18) |
| C24—O8 | 1.274 (3) | O3—H3B | 0.8200 |
| C25—C30 | 1.380 (4) | O3W—H3WB | 0.85 (4) |
| C25—C26 | 1.388 (4) | O3W—H3WA | 0.84 (4) |
| C25—C31 | 1.507 (4) | O6—H6B | 0.8200 |
| C26—C27 | 1.386 (4) | O9—H9A | 0.8200 |
| C26—H26A | 0.9300 | O12—H12A | 0.8200 |
| C27—C28 | 1.371 (4) | O15—H15C | 0.8200 |
| C27—H27A | 0.9300 | O18—H18B | 0.8200 |
| O5—Sm1—O4 | 53.20 (6) | C17—C18—H18A | 119.2 |
| O5—Sm1—O1W | 145.23 (6) | C18—C19—C20 | 119.3 (3) |
| O4—Sm1—O1W | 150.49 (7) | C18—C19—H19A | 120.3 |
| O5—Sm1—O10 | 73.25 (6) | C20—C19—H19A | 120.3 |
| O4—Sm1—O10 | 126.11 (6) | O9—C20—C21 | 118.2 (3) |
| O1W—Sm1—O10 | 79.74 (6) | O9—C20—C19 | 122.0 (3) |
| O5—Sm1—O2 | 123.26 (7) | C21—C20—C19 | 119.8 (3) |
| O4—Sm1—O2 | 116.84 (7) | C20—C21—C22 | 119.9 (3) |
| O1W—Sm1—O2 | 74.90 (7) | C20—C21—H21A | 120.0 |
| O10—Sm1—O2 | 85.59 (6) | C22—C21—H21A | 120.0 |
| O5—Sm1—O7 | 95.18 (7) | C17—C22—C21 | 121.4 (3) |
| O4—Sm1—O7 | 77.29 (7) | C17—C22—H22A | 119.3 |
| O1W—Sm1—O7 | 77.80 (8) | C21—C22—H22A | 119.3 |
| O10—Sm1—O7 | 116.92 (6) | C24—C23—C17 | 112.3 (3) |
| O2—Sm1—O7 | 140.51 (7) | C24—C23—H23A | 109.2 |
| O5—Sm1—O1 | 75.97 (7) | C17—C23—H23A | 109.2 |
| O4—Sm1—O1 | 72.89 (8) | C24—C23—H23B | 109.2 |
| O1W—Sm1—O1 | 126.25 (8) | C17—C23—H23B | 109.2 |

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| O10—Sm1—O1 | 90.25 (6) | H23A—C23—H23B | 107.9 |
| O2—Sm1—O1 | 51.61 (7) | O7—C24—O8 | 120.4 (2) |
| O7—Sm1—O1 | 148.06 (7) | O7—C24—C23 | 120.4 (2) |
| O5—Sm1—O8 | 75.80 (6) | O8—C24—C23 | 119.2 (3) |
| O4—Sm1—O8 | 102.16 (7) | O7—C24—Sm1 | 57.66 (14) |
| O1W—Sm1—O8 | 73.48 (7) | O8—C24—Sm1 | 63.20 (14) |
| O10—Sm1—O8 | 66.26 (6) | C23—C24—Sm1 | 171.2 (2) |
| O2—Sm1—O8 | 140.65 (6) | C30—C25—C26 | 118.0 (3) |
| O7—Sm1—O8 | 50.96 (6) | C30—C25—C31 | 120.3 (3) |
| O1—Sm1—O8 | 147.46 (6) | C26—C25—C31 | 121.7 (3) |
| O5—Sm1—N1 | 129.77 (7) | C27—C26—C25 | 121.0 (3) |
| O4—Sm1—N1 | 76.68 (7) | C27—C26—H26A | 119.5 |
| O1W—Sm1—N1 | 81.72 (7) | C25—C26—H26A | 119.5 |
| O10—Sm1—N1 | 155.06 (7) | C28—C27—C26 | 119.8 (3) |
| O2—Sm1—N1 | 73.54 (7) | C28—C27—H27A | 120.1 |
| O7—Sm1—N1 | 74.76 (7) | C26—C27—H27A | 120.1 |
| O1—Sm1—N1 | 87.38 (7) | C27—C28—O12 | 122.4 (3) |
| O8—Sm1—N1 | 123.48 (6) | C27—C28—C29 | 120.0 (3) |
| O5—Sm1—C16 | 26.79 (7) | O12—C28—C29 | 117.6 (3) |
| O4—Sm1—C16 | 26.63 (7) | C30—C29—C28 | 119.7 (3) |
| O1W—Sm1—C16 | 163.53 (8) | C30—C29—H29A | 120.1 |
| O10—Sm1—C16 | 99.49 (7) | C28—C29—H29A | 120.1 |
| O2—Sm1—C16 | 121.54 (8) | C29—C30—C25 | 121.4 (3) |
| O7—Sm1—C16 | 88.13 (8) | C29—C30—H30A | 119.3 |
| O1—Sm1—C16 | 70.06 (8) | C25—C30—H30A | 119.3 |
| O8—Sm1—C16 | 91.05 (7) | C25—C31—C32 | 114.9 (2) |
| N1—Sm1—C16 | 102.98 (8) | C25—C31—H31A | 108.5 |
| O5—Sm1—C8 | 100.86 (8) | C32—C31—H31A | 108.5 |
| O4—Sm1—C8 | 93.91 (8) | C25—C31—H31B | 108.5 |
| O1W—Sm1—C8 | 100.65 (9) | C32—C31—H31B | 108.5 |
| O10—Sm1—C8 | 90.08 (7) | H31A—C31—H31B | 107.5 |
| O2—Sm1—C8 | 25.75 (8) | O11—C32—O10 | 119.6 (2) |
| O7—Sm1—C8 | 151.75 (7) | O11—C32—C31 | 122.7 (2) |
| O1—Sm1—C8 | 26.07 (8) | O10—C32—C31 | 117.7 (2) |
| O8—Sm1—C8 | 156.18 (6) | O11—C32—Sm2 | 61.23 (14) |
| N1—Sm1—C8 | 77.11 (7) | O10—C32—Sm2 | 59.60 (13) |
| C16—Sm1—C8 | 95.79 (9) | C31—C32—Sm2 | 168.4 (2) |
| O5—Sm1—C24 | 86.95 (8) | C38—C33—C34 | 117.3 (2) |
| O4—Sm1—C24 | 91.04 (8) | C38—C33—C39 | 121.8 (3) |
| O1W—Sm1—C24 | 72.29 (8) | C34—C33—C39 | 120.9 (3) |
| O10—Sm1—C24 | 91.89 (7) | C35—C34—C33 | 121.4 (3) |
| O2—Sm1—C24 | 147.01 (8) | C35—C34—H34A | 119.3 |
| O7—Sm1—C24 | 25.05 (7) | C33—C34—H34A | 119.3 |
| O1—Sm1—C24 | 161.38 (8) | C34—C35—C36 | 120.5 (3) |
| O8—Sm1—C24 | 26.03 (6) | C34—C35—H35A | 119.7 |
| N1—Sm1—C24 | 98.21 (7) | C36—C35—H35A | 119.7 |
| C16—Sm1—C24 | 91.34 (8) | O15—C36—C37 | 123.0 (3) |
| C8—Sm1—C24 | 172.18 (8) | O15—C36—C35 | 117.9 (3) |
| O8—Sm2—O14 | 127.89 (6) | C37—C36—C35 | 119.0 (3) |

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| O8—Sm2—O13 | 75.13 (6) | C36—C37—C38 | 119.9 (3) |
| O14—Sm2—O13 | 53.27 (6) | C36—C37—H37A | 120.1 |
| O8—Sm2—O2W | 78.76 (7) | C38—C37—H37A | 120.1 |
| O14—Sm2—O2W | 143.94 (7) | C33—C38—C37 | 121.8 (3) |
| O13—Sm2—O2W | 147.65 (7) | C33—C38—H38A | 119.1 |
| O8—Sm2—O16 | 81.26 (6) | C37—C38—H38A | 119.1 |
| O14—Sm2—O16 | 126.48 (7) | C40—C39—C33 | 115.7 (2) |
| O13—Sm2—O16 | 117.96 (7) | C40—C39—H39A | 108.4 |
| O2W—Sm2—O16 | 75.82 (8) | C33—C39—H39A | 108.4 |
| O8—Sm2—O17 | 98.20 (7) | C40—C39—H39B | 108.4 |
| O14—Sm2—O17 | 77.89 (7) | C33—C39—H39B | 108.4 |
| O13—Sm2—O17 | 76.05 (7) | H39A—C39—H39B | 107.4 |
| O2W—Sm2—O17 | 126.91 (7) | O14—C40—O13 | 119.7 (3) |
| O16—Sm2—O17 | 51.67 (7) | O14—C40—C39 | 119.0 (2) |
| O8—Sm2—O10 | 67.51 (6) | O13—C40—C39 | 121.4 (2) |
| O14—Sm2—O10 | 90.92 (7) | O14—C40—Sm2 | 59.52 (14) |
| O13—Sm2—O10 | 75.70 (6) | O13—C40—Sm2 | 60.16 (14) |
| O2W—Sm2—O10 | 76.88 (7) | C39—C40—Sm2 | 177.20 (19) |
| O16—Sm2—O10 | 141.76 (6) | C42—C41—C46 | 117.7 (3) |
| O17—Sm2—O10 | 150.83 (6) | C42—C41—C47 | 122.1 (3) |
| O8—Sm2—O11 | 115.29 (6) | C46—C41—C47 | 120.2 (3) |
| O14—Sm2—O11 | 73.46 (7) | C43—C42—C41 | 121.9 (3) |
| O13—Sm2—O11 | 101.66 (7) | C43—C42—H42A | 119.0 |
| O2W—Sm2—O11 | 72.75 (7) | C41—C42—H42A | 119.0 |
| O16—Sm2—O11 | 140.11 (7) | C44—C43—C42 | 119.6 (3) |
| O17—Sm2—O11 | 144.90 (7) | C44—C43—H43A | 120.2 |
| O10—Sm2—O11 | 50.14 (5) | C42—C43—H43A | 120.2 |
| O8—Sm2—N3 | 155.05 (7) | O18—C44—C43 | 117.5 (3) |
| O14—Sm2—N3 | 75.76 (7) | O18—C44—C45 | 122.6 (3) |
| O13—Sm2—N3 | 126.14 (7) | C43—C44—C45 | 119.9 (3) |
| O2W—Sm2—N3 | 84.29 (7) | C46—C45—C44 | 119.6 (3) |
| O16—Sm2—N3 | 76.90 (7) | C46—C45—H45A | 120.2 |
| O17—Sm2—N3 | 77.54 (7) | C44—C45—H45A | 120.2 |
| O10—Sm2—N3 | 126.09 (6) | C45—C46—C41 | 121.3 (3) |
| O11—Sm2—N3 | 76.13 (6) | C45—C46—H46A | 119.4 |
| O8—Sm2—C40 | 101.68 (7) | C41—C46—H46A | 119.4 |
| O14—Sm2—C40 | 26.53 (7) | C48—C47—C41 | 112.1 (2) |
| O13—Sm2—C40 | 26.75 (7) | C48—C47—H47A | 109.2 |
| O2W—Sm2—C40 | 157.91 (8) | C41—C47—H47A | 109.2 |
| O16—Sm2—C40 | 126.24 (8) | C48—C47—H47B | 109.2 |
| O17—Sm2—C40 | 75.11 (7) | C41—C47—H47B | 109.2 |
| O10—Sm2—C40 | 82.88 (7) | H47A—C47—H47B | 107.9 |
| O11—Sm2—C40 | 87.53 (7) | O16—C48—O17 | 119.5 (3) |
| N3—Sm2—C40 | 100.89 (7) | O16—C48—C47 | 120.3 (3) |
| O8—Sm2—C48 | 91.70 (7) | O17—C48—C47 | 120.2 (3) |
| O14—Sm2—C48 | 101.89 (9) | O16—C48—Sm2 | 58.51 (15) |
| O13—Sm2—C48 | 98.78 (8) | O17—C48—Sm2 | 61.67 (15) |
| O2W—Sm2—C48 | 100.77 (9) | C47—C48—Sm2 | 171.01 (19) |
| O16—Sm2—C48 | 25.63 (8) | N1—C49—C50 | 123.3 (3) |

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| O17—Sm2—C48 | 26.22 (8) | N1—C49—H49A | 118.4 |
| O10—Sm2—C48 | 159.18 (7) | C50—C49—H49A | 118.4 |
| O11—Sm2—C48 | 149.49 (7) | C49—C50—C51 | 119.9 (3) |
| N3—Sm2—C48 | 73.54 (7) | C49—C50—H50A | 120.1 |
| C40—Sm2—C48 | 101.29 (9) | C51—C50—H50A | 120.1 |
| O8—Sm2—C32 | 90.76 (6) | C50—C51—C52 | 116.9 (2) |
| O14—Sm2—C32 | 84.15 (8) | C50—C51—C56 | 121.4 (3) |
| O13—Sm2—C32 | 91.20 (7) | C52—C51—C56 | 121.7 (3) |
| O2W—Sm2—C32 | 70.24 (8) | C53—C52—C51 | 119.8 (3) |
| O16—Sm2—C32 | 146.03 (8) | C53—C52—H52A | 120.1 |
| O17—Sm2—C32 | 161.85 (8) | C51—C52—H52A | 120.1 |
| O10—Sm2—C32 | 25.46 (6) | N1—C53—C52 | 123.5 (3) |
| O11—Sm2—C32 | 25.00 (6) | N1—C53—H53A | 118.2 |
| N3—Sm2—C32 | 100.64 (7) | C52—C53—H53A | 118.2 |
| C40—Sm2—C32 | 87.67 (8) | N2—C54—C55 | 124.2 (4) |
| C48—Sm2—C32 | 170.02 (8) | N2—C54—H54A | 117.9 |
| C53—N1—C49 | 116.6 (2) | C55—C54—H54A | 117.9 |
| C53—N1—Sm1 | 118.68 (18) | C54—C55—C56 | 119.2 (4) |
| C49—N1—Sm1 | 124.39 (18) | C54—C55—H55A | 120.4 |
| C58—N2—C54 | 115.9 (3) | C56—C55—H55A | 120.4 |
| C63—N3—C59 | 116.5 (2) | C57—C56—C55 | 116.8 (3) |
| C63—N3—Sm2 | 121.64 (18) | C57—C56—C51 | 122.0 (3) |
| C59—N3—Sm2 | 121.42 (18) | C55—C56—C51 | 121.1 (3) |
| C64—N4—C68 | 116.2 (3) | C56—C57—C58 | 119.6 (4) |
| C2—C1—C6 | 117.5 (3) | C56—C57—H57A | 120.2 |
| C2—C1—C7 | 122.4 (3) | C58—C57—H57A | 120.2 |
| C6—C1—C7 | 120.1 (3) | N2—C58—C57 | 124.2 (4) |
| C1—C2—C3 | 121.5 (3) | N2—C58—H58A | 117.9 |
| C1—C2—H2A | 119.3 | C57—C58—H58A | 117.9 |
| C3—C2—H2A | 119.3 | N3—C59—C60 | 123.1 (3) |
| C4—C3—C2 | 119.8 (3) | N3—C59—H59A | 118.4 |
| C4—C3—H3A | 120.1 | C60—C59—H59A | 118.4 |
| C2—C3—H3A | 120.1 | C59—C60—C61 | 120.3 (3) |
| C3—C4—C5 | 119.7 (3) | C59—C60—H60A | 119.9 |
| C3—C4—O3 | 118.5 (3) | C61—C60—H60A | 119.9 |
| C5—C4—O3 | 121.8 (3) | C60—C61—C62 | 116.4 (2) |
| C4—C5—C6 | 120.3 (3) | C60—C61—C66 | 120.8 (3) |
| C4—C5—H5A | 119.9 | C62—C61—C66 | 122.7 (3) |
| C6—C5—H5A | 119.9 | C63—C62—C61 | 120.2 (3) |
| C5—C6—C1 | 121.2 (3) | C63—C62—H62A | 119.9 |
| C5—C6—H6A | 119.4 | C61—C62—H62A | 119.9 |
| C1—C6—H6A | 119.4 | N3—C63—C62 | 123.2 (3) |
| C8—C7—C1 | 111.8 (2) | N3—C63—H63A | 118.4 |
| C8—C7—H7A | 109.3 | C62—C63—H63A | 118.4 |
| C1—C7—H7A | 109.3 | N4—C64—C65 | 124.0 (4) |
| C8—C7—H7B | 109.3 | N4—C64—H64A | 118.0 |
| C1—C7—H7B | 109.3 | C65—C64—H64A | 118.0 |
| H7A—C7—H7B | 107.9 | C64—C65—C66 | 119.7 (4) |
| O1—C8—O2 | 119.4 (3) | C64—C65—H65A | 120.2 |

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| O1—C8—C7 | 120.7 (3) | C66—C65—H65A | 120.2 |
| O2—C8—C7 | 119.9 (3) | C65—C66—C67 | 116.8 (3) |
| O1—C8—Sm1 | 62.24 (15) | C65—C66—C61 | 122.2 (3) |
| O2—C8—Sm1 | 57.91 (15) | C67—C66—C61 | 120.9 (3) |
| C7—C8—Sm1 | 169.06 (18) | C68—C67—C66 | 118.9 (4) |
| C10—C9—C14 | 117.2 (3) | C68—C67—H67A | 120.5 |
| C10—C9—C15 | 121.7 (3) | C66—C67—H67A | 120.5 |
| C14—C9—C15 | 121.1 (3) | N4—C68—C67 | 124.4 (4) |
| C9—C10—C11 | 122.1 (3) | N4—C68—H68A | 117.8 |
| C9—C10—H10A | 119.0 | C67—C68—H68A | 117.8 |
| C11—C10—H10A | 119.0 | Sm1—O1W—H1WA | 116 (3) |
| C12—C11—C10 | 119.1 (3) | Sm1—O1W—H1WB | 138 (3) |
| C12—C11—H11A | 120.5 | H1WA—O1W—H1WB | 105 (3) |
| C10—C11—H11A | 120.5 | C8—O1—Sm1 | 91.69 (17) |
| C13—C12—C11 | 119.9 (3) | Sm2—O2W—H2WA | 125 (3) |
| C13—C12—O6 | 117.5 (3) | Sm2—O2W—H2WB | 130 (3) |
| C11—C12—O6 | 122.6 (3) | H2WA—O2W—H2WB | 105 (3) |
| C12—C13—C14 | 120.2 (3) | C8—O2—Sm1 | 96.34 (18) |
| C12—C13—H13A | 119.9 | C4—O3—H3B | 109.5 |
| C14—C13—H13A | 119.9 | H3WB—O3W—H3WA | 102 (3) |
| C13—C14—C9 | 121.5 (3) | C16—O4—Sm1 | 92.64 (17) |
| C13—C14—H14A | 119.3 | C16—O5—Sm1 | 92.66 (16) |
| C9—C14—H14A | 119.3 | C12—O6—H6B | 109.5 |
| C9—C15—C16 | 114.9 (2) | C24—O7—Sm1 | 97.28 (16) |
| C9—C15—H15A | 108.5 | C24—O8—Sm2 | 153.69 (18) |
| C16—C15—H15A | 108.5 | C24—O8—Sm1 | 90.77 (15) |
| C9—C15—H15B | 108.5 | Sm2—O8—Sm1 | 113.39 (7) |
| C16—C15—H15B | 108.5 | C20—O9—H9A | 109.5 |
| H15A—C15—H15B | 107.5 | C32—O10—Sm1 | 142.67 (17) |
| O4—C16—O5 | 120.5 (3) | C32—O10—Sm2 | 94.93 (15) |
| O4—C16—C15 | 118.7 (3) | Sm1—O10—Sm2 | 112.84 (6) |
| O5—C16—C15 | 120.7 (2) | C32—O11—Sm2 | 93.77 (15) |
| O4—C16—Sm1 | 60.73 (15) | C28—O12—H12A | 109.5 |
| O5—C16—Sm1 | 60.56 (14) | C40—O13—Sm2 | 93.09 (15) |
| C15—C16—Sm1 | 169.1 (2) | C40—O14—Sm2 | 93.95 (16) |
| C22—C17—C18 | 117.9 (3) | C36—O15—H15C | 109.5 |
| C22—C17—C23 | 121.1 (3) | C48—O16—Sm2 | 95.86 (18) |
| C18—C17—C23 | 121.0 (3) | C48—O17—Sm2 | 92.11 (18) |
| C19—C18—C17 | 121.7 (3) | C44—O18—H18B | 109.5 |
| C19—C18—H18A | 119.2 | | |
| O5—Sm1—N1—C53 | 41.9 (3) | O13—Sm2—C48—O17 | -30.02 (17) |
| O4—Sm1—N1—C53 | 38.2 (2) | O2W—Sm2—C48—O17 | 175.88 (16) |
| O1W—Sm1—N1—C53 | -121.6 (2) | O16—Sm2—C48—O17 | -170.8 (3) |
| O10—Sm1—N1—C53 | -163.8 (2) | O10—Sm2—C48—O17 | -102.7 (3) |
| O2—Sm1—N1—C53 | 161.8 (2) | O11—Sm2—C48—O17 | 101.6 (2) |
| O7—Sm1—N1—C53 | -42.0 (2) | N3—Sm2—C48—O17 | 95.19 (17) |
| O1—Sm1—N1—C53 | 111.2 (2) | C40—Sm2—C48—O17 | -2.97 (18) |
| O8—Sm1—N1—C53 | -57.7 (2) | C53—N1—C49—C50 | 2.0 (5) |
| C16—Sm1—N1—C53 | 42.4 (2) | Sm1—N1—C49—C50 | -171.2 (2) |

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|----------------|-------------|-----------------|--------------|
| C8—Sm1—N1—C53 | 135.4 (2) | N1—C49—C50—C51 | 0.1 (5) |
| C24—Sm1—N1—C53 | -50.9 (2) | C49—C50—C51—C52 | -2.1 (5) |
| O5—Sm1—N1—C49 | -145.0 (2) | C49—C50—C51—C56 | 176.2 (3) |
| O4—Sm1—N1—C49 | -148.7 (2) | C50—C51—C52—C53 | 1.9 (5) |
| O1W—Sm1—N1—C49 | 51.5 (2) | C56—C51—C52—C53 | -176.5 (3) |
| O10—Sm1—N1—C49 | 9.2 (3) | C49—N1—C53—C52 | -2.3 (5) |
| O2—Sm1—N1—C49 | -25.1 (2) | Sm1—N1—C53—C52 | 171.4 (3) |
| O7—Sm1—N1—C49 | 131.0 (2) | C51—C52—C53—N1 | 0.3 (5) |
| O1—Sm1—N1—C49 | -75.7 (2) | C58—N2—C54—C55 | 1.1 (6) |
| O8—Sm1—N1—C49 | 115.4 (2) | N2—C54—C55—C56 | -0.5 (6) |
| C16—Sm1—N1—C49 | -144.6 (2) | C54—C55—C56—C57 | -1.2 (5) |
| C8—Sm1—N1—C49 | -51.5 (2) | C54—C55—C56—C51 | 176.2 (3) |
| C24—Sm1—N1—C49 | 122.1 (2) | C50—C51—C56—C57 | 29.0 (5) |
| O8—Sm2—N3—C63 | 173.16 (19) | C52—C51—C56—C57 | -152.8 (3) |
| O14—Sm2—N3—C63 | -23.8 (2) | C50—C51—C56—C55 | -148.3 (3) |
| O13—Sm2—N3—C63 | -42.1 (2) | C52—C51—C56—C55 | 30.0 (5) |
| O2W—Sm2—N3—C63 | 125.9 (2) | C55—C56—C57—C58 | 2.2 (6) |
| O16—Sm2—N3—C63 | -157.3 (2) | C51—C56—C57—C58 | -175.1 (3) |
| O17—Sm2—N3—C63 | -104.2 (2) | C54—N2—C58—C57 | 0.0 (6) |
| O10—Sm2—N3—C63 | 56.8 (2) | C56—C57—C58—N2 | -1.7 (7) |
| O11—Sm2—N3—C63 | 52.3 (2) | C63—N3—C59—C60 | -2.1 (4) |
| C40—Sm2—N3—C63 | -32.3 (2) | Sm2—N3—C59—C60 | 170.8 (2) |
| C48—Sm2—N3—C63 | -131.0 (2) | N3—C59—C60—C61 | -1.5 (5) |
| C32—Sm2—N3—C63 | 57.3 (2) | C59—C60—C61—C62 | 3.5 (4) |
| O8—Sm2—N3—C59 | 0.6 (3) | C59—C60—C61—C66 | -173.5 (3) |
| O14—Sm2—N3—C59 | 163.7 (2) | C60—C61—C62—C63 | -2.2 (4) |
| O13—Sm2—N3—C59 | 145.3 (2) | C66—C61—C62—C63 | 174.8 (3) |
| O2W—Sm2—N3—C59 | -46.6 (2) | C59—N3—C63—C62 | 3.6 (4) |
| O16—Sm2—N3—C59 | 30.1 (2) | Sm2—N3—C63—C62 | -169.3 (2) |
| O17—Sm2—N3—C59 | 83.2 (2) | C61—C62—C63—N3 | -1.5 (5) |
| O10—Sm2—N3—C59 | -115.8 (2) | C68—N4—C64—C65 | -0.3 (6) |
| O11—Sm2—N3—C59 | -120.2 (2) | N4—C64—C65—C66 | 2.5 (6) |
| C40—Sm2—N3—C59 | 155.1 (2) | C64—C65—C66—C67 | -2.4 (5) |
| C48—Sm2—N3—C59 | 56.4 (2) | C64—C65—C66—C61 | 174.5 (3) |
| C32—Sm2—N3—C59 | -115.2 (2) | C60—C61—C66—C65 | -17.0 (5) |
| C6—C1—C2—C3 | -1.1 (5) | C62—C61—C66—C65 | 166.1 (3) |
| C7—C1—C2—C3 | -179.2 (3) | C60—C61—C66—C67 | 159.7 (3) |
| C1—C2—C3—C4 | 0.4 (5) | C62—C61—C66—C67 | -17.1 (5) |
| C2—C3—C4—C5 | 1.4 (5) | C65—C66—C67—C68 | 0.4 (5) |
| C2—C3—C4—O3 | -179.5 (3) | C61—C66—C67—C68 | -176.5 (3) |
| C3—C4—C5—C6 | -2.5 (5) | C64—N4—C68—C67 | -1.9 (6) |
| O3—C4—C5—C6 | 178.4 (3) | C66—C67—C68—N4 | 1.9 (6) |
| C4—C5—C6—C1 | 1.8 (5) | O2—C8—O1—Sm1 | 9.7 (3) |
| C2—C1—C6—C5 | 0.0 (5) | C7—C8—O1—Sm1 | -167.9 (2) |
| C7—C1—C6—C5 | 178.2 (3) | O5—Sm1—O1—C8 | -162.32 (17) |
| C2—C1—C7—C8 | -48.6 (4) | O4—Sm1—O1—C8 | 142.36 (17) |
| C6—C1—C7—C8 | 133.4 (3) | O1W—Sm1—O1—C8 | -12.25 (19) |
| C1—C7—C8—O1 | 99.3 (3) | O10—Sm1—O1—C8 | -89.67 (16) |
| C1—C7—C8—O2 | -78.3 (3) | O2—Sm1—O1—C8 | -5.50 (15) |

supplementary materials

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| C1—C7—C8—Sm1 | -3.1 (14) | O7—Sm1—O1—C8 | 120.68 (18) |
| O5—Sm1—C8—O1 | 17.46 (17) | O8—Sm1—O1—C8 | -131.82 (16) |
| O4—Sm1—C8—O1 | -35.80 (16) | N1—Sm1—O1—C8 | 65.50 (16) |
| O1W—Sm1—C8—O1 | 169.98 (16) | C16—Sm1—O1—C8 | 170.32 (18) |
| O10—Sm1—C8—O1 | 90.41 (16) | C24—Sm1—O1—C8 | 173.7 (2) |
| O2—Sm1—C8—O1 | 170.0 (3) | O1—C8—O2—Sm1 | -10.1 (3) |
| O7—Sm1—C8—O1 | -106.0 (2) | C7—C8—O2—Sm1 | 167.5 (2) |
| O8—Sm1—C8—O1 | 96.9 (2) | O5—Sm1—O2—C8 | 32.73 (18) |
| N1—Sm1—C8—O1 | -111.17 (17) | O4—Sm1—O2—C8 | -29.18 (17) |
| C16—Sm1—C8—O1 | -9.14 (17) | O1W—Sm1—O2—C8 | 179.93 (17) |
| O5—Sm1—C8—O2 | -152.59 (15) | O10—Sm1—O2—C8 | 99.38 (16) |
| O4—Sm1—C8—O2 | 154.15 (15) | O7—Sm1—O2—C8 | -132.26 (16) |
| O1W—Sm1—C8—O2 | -0.07 (16) | O1—Sm1—O2—C8 | 5.56 (15) |
| O10—Sm1—C8—O2 | -79.64 (16) | O8—Sm1—O2—C8 | 142.44 (15) |
| O7—Sm1—C8—O2 | 83.9 (2) | N1—Sm1—O2—C8 | -94.42 (16) |
| O1—Sm1—C8—O2 | -170.0 (3) | C16—Sm1—O2—C8 | 0.94 (18) |
| O8—Sm1—C8—O2 | -73.2 (2) | C24—Sm1—O2—C8 | -173.95 (15) |
| N1—Sm1—C8—O2 | 78.78 (16) | O5—C16—O4—Sm1 | 9.9 (3) |
| C16—Sm1—C8—O2 | -179.19 (16) | C15—C16—O4—Sm1 | -167.6 (3) |
| O5—Sm1—C8—C7 | 125.7 (12) | O5—Sm1—O4—C16 | -5.52 (16) |
| O4—Sm1—C8—C7 | 72.5 (12) | O1W—Sm1—O4—C16 | -145.07 (18) |
| O1W—Sm1—C8—C7 | -81.8 (12) | O10—Sm1—O4—C16 | 2.2 (2) |
| O10—Sm1—C8—C7 | -161.3 (12) | O2—Sm1—O4—C16 | 107.38 (18) |
| O2—Sm1—C8—C7 | -81.7 (12) | O7—Sm1—O4—C16 | -112.04 (18) |
| O7—Sm1—C8—C7 | 2.3 (13) | O1—Sm1—O4—C16 | 79.52 (18) |
| O1—Sm1—C8—C7 | 108.3 (13) | O8—Sm1—O4—C16 | -67.19 (18) |
| O8—Sm1—C8—C7 | -154.9 (11) | N1—Sm1—O4—C16 | 170.88 (19) |
| N1—Sm1—C8—C7 | -2.9 (12) | C8—Sm1—O4—C16 | 95.12 (18) |
| C16—Sm1—C8—C7 | 99.1 (12) | C24—Sm1—O4—C16 | -90.93 (18) |
| C14—C9—C10—C11 | 0.4 (5) | O4—C16—O5—Sm1 | -10.0 (3) |
| C15—C9—C10—C11 | -179.1 (3) | C15—C16—O5—Sm1 | 167.5 (3) |
| C9—C10—C11—C12 | -0.1 (5) | O4—Sm1—O5—C16 | 5.49 (16) |
| C10—C11—C12—C13 | -0.8 (5) | O1W—Sm1—O5—C16 | 151.41 (17) |
| C10—C11—C12—O6 | 179.1 (3) | O10—Sm1—O5—C16 | -168.04 (18) |
| C11—C12—C13—C14 | 1.3 (5) | O2—Sm1—O5—C16 | -95.10 (17) |
| O6—C12—C13—C14 | -178.6 (3) | O7—Sm1—O5—C16 | 75.38 (17) |
| C12—C13—C14—C9 | -1.0 (5) | O1—Sm1—O5—C16 | -73.45 (17) |
| C10—C9—C14—C13 | 0.1 (5) | O8—Sm1—O5—C16 | 122.91 (17) |
| C15—C9—C14—C13 | 179.6 (3) | N1—Sm1—O5—C16 | 0.9 (2) |
| C10—C9—C15—C16 | -99.8 (4) | C8—Sm1—O5—C16 | -81.26 (17) |
| C14—C9—C15—C16 | 80.6 (4) | C24—Sm1—O5—C16 | 99.07 (17) |
| C9—C15—C16—O4 | 172.7 (3) | O8—C24—O7—Sm1 | -7.9 (3) |
| C9—C15—C16—O5 | -4.9 (4) | C23—C24—O7—Sm1 | 170.0 (3) |
| C9—C15—C16—Sm1 | 88.5 (10) | O5—Sm1—O7—C24 | 71.33 (19) |
| O5—Sm1—C16—O4 | 170.2 (3) | O4—Sm1—O7—C24 | 121.8 (2) |
| O1W—Sm1—C16—O4 | 95.9 (3) | O1W—Sm1—O7—C24 | -74.19 (19) |
| O10—Sm1—C16—O4 | -178.23 (17) | O10—Sm1—O7—C24 | -2.5 (2) |
| O2—Sm1—C16—O4 | -87.59 (18) | O2—Sm1—O7—C24 | -121.23 (19) |
| O7—Sm1—C16—O4 | 64.78 (18) | O1—Sm1—O7—C24 | 142.98 (18) |

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| O1—Sm1—C16—O4 | -91.43 (18) | O8—Sm1—O7—C24 | 4.32 (17) |
| O8—Sm1—C16—O4 | 115.67 (18) | N1—Sm1—O7—C24 | -158.8 (2) |
| N1—Sm1—C16—O4 | -9.11 (19) | C16—Sm1—O7—C24 | 97.2 (2) |
| C8—Sm1—C16—O4 | -87.17 (18) | C8—Sm1—O7—C24 | -164.0 (2) |
| C24—Sm1—C16—O4 | 89.63 (18) | O7—C24—O8—Sm2 | 164.8 (3) |
| O4—Sm1—C16—O5 | -170.2 (3) | C23—C24—O8—Sm2 | -13.1 (6) |
| O1W—Sm1—C16—O5 | -74.3 (3) | Sm1—C24—O8—Sm2 | 157.3 (4) |
| O10—Sm1—C16—O5 | 11.61 (17) | O7—C24—O8—Sm1 | 7.5 (3) |
| O2—Sm1—C16—O5 | 102.25 (17) | C23—C24—O8—Sm1 | -170.4 (3) |
| O7—Sm1—C16—O5 | -105.38 (17) | O14—Sm2—O8—C24 | -82.6 (4) |
| O1—Sm1—C16—O5 | 98.40 (17) | O13—Sm2—O8—C24 | -74.7 (4) |
| O8—Sm1—C16—O5 | -54.49 (17) | O2W—Sm2—O8—C24 | 124.6 (4) |
| N1—Sm1—C16—O5 | -179.27 (16) | O16—Sm2—O8—C24 | 47.4 (4) |
| C8—Sm1—C16—O5 | 102.66 (17) | O17—Sm2—O8—C24 | -1.6 (4) |
| C24—Sm1—C16—O5 | -80.53 (17) | O10—Sm2—O8—C24 | -155.1 (4) |
| O5—Sm1—C16—C15 | -99.6 (10) | O11—Sm2—O8—C24 | -170.8 (4) |
| O4—Sm1—C16—C15 | 90.2 (10) | N3—Sm2—O8—C24 | 76.5 (5) |
| O1W—Sm1—C16—C15 | -173.9 (9) | C40—Sm2—O8—C24 | -78.0 (4) |
| O10—Sm1—C16—C15 | -88.0 (10) | C48—Sm2—O8—C24 | 23.9 (4) |
| O2—Sm1—C16—C15 | 2.7 (10) | C32—Sm2—O8—C24 | -165.7 (4) |
| O7—Sm1—C16—C15 | 155.0 (10) | O14—Sm2—O8—Sm1 | 72.61 (11) |
| O1—Sm1—C16—C15 | -1.2 (10) | O13—Sm2—O8—Sm1 | 80.48 (8) |
| O8—Sm1—C16—C15 | -154.1 (10) | O2W—Sm2—O8—Sm1 | -80.24 (9) |
| N1—Sm1—C16—C15 | 81.1 (10) | O16—Sm2—O8—Sm1 | -157.40 (9) |
| C8—Sm1—C16—C15 | 3.1 (10) | O17—Sm2—O8—Sm1 | 153.60 (8) |
| C24—Sm1—C16—C15 | 179.7 (12) | O10—Sm2—O8—Sm1 | 0.08 (6) |
| C22—C17—C18—C19 | 0.3 (4) | O11—Sm2—O8—Sm1 | -15.60 (10) |
| C23—C17—C18—C19 | 178.9 (3) | N3—Sm2—O8—Sm1 | -128.35 (14) |
| C17—C18—C19—C20 | 0.0 (5) | C40—Sm2—O8—Sm1 | 77.21 (9) |
| C18—C19—C20—O9 | -180.0 (3) | C48—Sm2—O8—Sm1 | 179.11 (9) |
| C18—C19—C20—C21 | -0.5 (5) | C32—Sm2—O8—Sm1 | -10.57 (9) |
| O9—C20—C21—C22 | -179.9 (3) | O5—Sm1—O8—C24 | -113.14 (17) |
| C19—C20—C21—C22 | 0.6 (5) | O4—Sm1—O8—C24 | -66.49 (17) |
| C18—C17—C22—C21 | -0.2 (5) | O1W—Sm1—O8—C24 | 83.36 (17) |
| C23—C17—C22—C21 | -178.8 (3) | O10—Sm1—O8—C24 | 169.19 (18) |
| C20—C21—C22—C17 | -0.2 (5) | O2—Sm1—O8—C24 | 121.15 (17) |
| C22—C17—C23—C24 | 98.0 (4) | O7—Sm1—O8—C24 | -4.17 (17) |
| C18—C17—C23—C24 | -80.5 (4) | O1—Sm1—O8—C24 | -143.66 (18) |
| C17—C23—C24—O7 | -45.2 (5) | N1—Sm1—O8—C24 | 15.45 (19) |
| C17—C23—C24—O8 | 132.7 (3) | C16—Sm1—O8—C24 | -90.90 (17) |
| O5—Sm1—C24—O7 | -109.12 (19) | C8—Sm1—O8—C24 | 162.1 (2) |
| O4—Sm1—C24—O7 | -56.05 (19) | O5—Sm1—O8—Sm2 | 77.59 (8) |
| O1W—Sm1—C24—O7 | 99.17 (19) | O4—Sm1—O8—Sm2 | 124.24 (8) |
| O10—Sm1—C24—O7 | 177.77 (19) | O1W—Sm1—O8—Sm2 | -85.92 (9) |
| O2—Sm1—C24—O7 | 93.0 (2) | O10—Sm1—O8—Sm2 | -0.08 (7) |
| O1—Sm1—C24—O7 | -85.8 (3) | O2—Sm1—O8—Sm2 | -48.12 (13) |
| O8—Sm1—C24—O7 | -172.3 (3) | O7—Sm1—O8—Sm2 | -173.44 (12) |
| N1—Sm1—C24—O7 | 20.6 (2) | O1—Sm1—O8—Sm2 | 47.06 (16) |
| C16—Sm1—C24—O7 | -82.69 (19) | N1—Sm1—O8—Sm2 | -153.82 (8) |

supplementary materials

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| O5—Sm1—C24—O8 | 63.22 (16) | C16—Sm1—O8—Sm2 | 99.83 (9) |
| O4—Sm1—C24—O8 | 116.29 (16) | C8—Sm1—O8—Sm2 | -7.1 (2) |
| O1W—Sm1—C24—O8 | -88.49 (17) | C24—Sm1—O8—Sm2 | -169.3 (2) |
| O10—Sm1—C24—O8 | -9.89 (17) | O11—C32—O10—Sm1 | -151.8 (2) |
| O2—Sm1—C24—O8 | -94.70 (19) | C31—C32—O10—Sm1 | 28.0 (4) |
| O7—Sm1—C24—O8 | 172.3 (3) | Sm2—C32—O10—Sm1 | -139.1 (3) |
| O1—Sm1—C24—O8 | 86.5 (3) | O11—C32—O10—Sm2 | -12.7 (3) |
| N1—Sm1—C24—O8 | -167.03 (16) | C31—C32—O10—Sm2 | 167.1 (2) |
| C16—Sm1—C24—O8 | 89.66 (17) | O5—Sm1—O10—C32 | 53.5 (3) |
| C30—C25—C26—C27 | -1.0 (4) | O4—Sm1—O10—C32 | 47.1 (3) |
| C31—C25—C26—C27 | 177.9 (3) | O1W—Sm1—O10—C32 | -148.6 (3) |
| C25—C26—C27—C28 | -0.5 (5) | O2—Sm1—O10—C32 | -73.2 (3) |
| C26—C27—C28—O12 | -179.6 (3) | O7—Sm1—O10—C32 | 140.8 (3) |
| C26—C27—C28—C29 | 1.5 (5) | O1—Sm1—O10—C32 | -21.8 (3) |
| C27—C28—C29—C30 | -1.0 (5) | O8—Sm1—O10—C32 | 135.0 (3) |
| O12—C28—C29—C30 | -179.9 (3) | N1—Sm1—O10—C32 | -106.1 (3) |
| C28—C29—C30—C25 | -0.6 (5) | C16—Sm1—O10—C32 | 48.1 (3) |
| C26—C25—C30—C29 | 1.6 (5) | C8—Sm1—O10—C32 | -47.8 (3) |
| C31—C25—C30—C29 | -177.3 (3) | C24—Sm1—O10—C32 | 139.7 (3) |
| C30—C25—C31—C32 | 75.7 (4) | O5—Sm1—O10—Sm2 | -81.44 (8) |
| C26—C25—C31—C32 | -103.2 (3) | O4—Sm1—O10—Sm2 | -87.86 (10) |
| C25—C31—C32—O11 | 12.0 (5) | O1W—Sm1—O10—Sm2 | 76.42 (8) |
| C25—C31—C32—O10 | -167.8 (3) | O2—Sm1—O10—Sm2 | 151.85 (8) |
| C25—C31—C32—Sm2 | -94.3 (9) | O7—Sm1—O10—Sm2 | 5.86 (11) |
| O8—Sm2—C32—O11 | -169.19 (17) | O1—Sm1—O10—Sm2 | -156.70 (8) |
| O14—Sm2—C32—O11 | 62.78 (17) | O8—Sm1—O10—Sm2 | 0.07 (6) |
| O13—Sm2—C32—O11 | 115.67 (17) | N1—Sm1—O10—Sm2 | 118.99 (15) |
| O2W—Sm2—C32—O11 | -91.42 (18) | C16—Sm1—O10—Sm2 | -86.88 (9) |
| O16—Sm2—C32—O11 | -93.80 (19) | C8—Sm1—O10—Sm2 | 177.23 (9) |
| O17—Sm2—C32—O11 | 70.9 (3) | C24—Sm1—O10—Sm2 | 4.80 (9) |
| O10—Sm2—C32—O11 | 167.4 (3) | O8—Sm2—O10—C32 | -154.56 (18) |
| N3—Sm2—C32—O11 | -11.50 (18) | O14—Sm2—O10—C32 | 74.28 (16) |
| C40—Sm2—C32—O11 | 89.15 (17) | O13—Sm2—O10—C32 | 125.87 (17) |
| O8—Sm2—C32—O10 | 23.39 (16) | O2W—Sm2—O10—C32 | -71.46 (16) |
| O14—Sm2—C32—O10 | -104.64 (16) | O16—Sm2—O10—C32 | -116.85 (17) |
| O13—Sm2—C32—O10 | -51.76 (16) | O17—Sm2—O10—C32 | 140.59 (18) |
| O2W—Sm2—C32—O10 | 101.15 (16) | O11—Sm2—O10—C32 | 6.88 (16) |
| O16—Sm2—C32—O10 | 98.78 (18) | N3—Sm2—O10—C32 | 1.30 (19) |
| O17—Sm2—C32—O10 | -96.5 (3) | C40—Sm2—O10—C32 | 99.62 (17) |
| O11—Sm2—C32—O10 | -167.4 (3) | C48—Sm2—O10—C32 | -157.3 (2) |
| N3—Sm2—C32—O10 | -178.93 (15) | O8—Sm2—O10—Sm1 | -0.08 (7) |
| C40—Sm2—C32—O10 | -78.28 (16) | O14—Sm2—O10—Sm1 | -131.24 (8) |
| O8—Sm2—C32—C31 | -56.4 (9) | O13—Sm2—O10—Sm1 | -79.65 (8) |
| O14—Sm2—C32—C31 | 175.6 (9) | O2W—Sm2—O10—Sm1 | 83.02 (8) |
| O13—Sm2—C32—C31 | -131.5 (9) | O16—Sm2—O10—Sm1 | 37.63 (13) |
| O2W—Sm2—C32—C31 | 21.4 (9) | O17—Sm2—O10—Sm1 | -64.93 (16) |
| O16—Sm2—C32—C31 | 19.0 (10) | O11—Sm2—O10—Sm1 | 161.36 (12) |
| O17—Sm2—C32—C31 | -176.3 (8) | N3—Sm2—O10—Sm1 | 155.78 (8) |
| O10—Sm2—C32—C31 | -79.8 (9) | C40—Sm2—O10—Sm1 | -105.90 (8) |

| | | | |
|-----------------|--------------|-----------------|--------------|
| O11—Sm2—C32—C31 | 112.8 (10) | C48—Sm2—O10—Sm1 | -2.8 (3) |
| N3—Sm2—C32—C31 | 101.3 (9) | C32—Sm2—O10—Sm1 | 154.5 (2) |
| C40—Sm2—C32—C31 | -158.0 (9) | O10—C32—O11—Sm2 | 12.5 (3) |
| C38—C33—C34—C35 | -0.1 (5) | C31—C32—O11—Sm2 | -167.3 (3) |
| C39—C33—C34—C35 | 179.2 (3) | O8—Sm2—O11—C32 | 11.97 (19) |
| C33—C34—C35—C36 | -0.4 (5) | O14—Sm2—O11—C32 | -112.65 (18) |
| C34—C35—C36—O15 | -179.4 (3) | O13—Sm2—O11—C32 | -66.94 (18) |
| C34—C35—C36—C37 | 0.3 (5) | O2W—Sm2—O11—C32 | 80.11 (18) |
| O15—C36—C37—C38 | 179.9 (3) | O16—Sm2—O11—C32 | 119.63 (18) |
| C35—C36—C37—C38 | 0.2 (5) | O17—Sm2—O11—C32 | -149.20 (17) |
| C34—C33—C38—C37 | 0.6 (5) | O10—Sm2—O11—C32 | -7.00 (16) |
| C39—C33—C38—C37 | -178.7 (3) | N3—Sm2—O11—C32 | 168.36 (18) |
| C36—C37—C38—C33 | -0.6 (5) | C40—Sm2—O11—C32 | -89.78 (18) |
| C38—C33—C39—C40 | -114.4 (3) | C48—Sm2—O11—C32 | 161.98 (19) |
| C34—C33—C39—C40 | 66.3 (4) | O14—C40—O13—Sm2 | 1.1 (3) |
| C33—C39—C40—O14 | 173.8 (3) | C39—C40—O13—Sm2 | -177.3 (2) |
| C33—C39—C40—O13 | -7.8 (4) | O8—Sm2—O13—C40 | -172.88 (18) |
| O8—Sm2—C40—O14 | -171.84 (16) | O14—Sm2—O13—C40 | -0.63 (16) |
| O13—Sm2—C40—O14 | -178.9 (3) | O2W—Sm2—O13—C40 | -135.63 (18) |
| O2W—Sm2—C40—O14 | -83.0 (2) | O16—Sm2—O13—C40 | 115.71 (17) |
| O16—Sm2—C40—O14 | 100.50 (17) | O17—Sm2—O13—C40 | 84.53 (17) |
| O17—Sm2—C40—O14 | 92.67 (17) | O10—Sm2—O13—C40 | -102.81 (17) |
| O10—Sm2—C40—O14 | -106.64 (17) | O11—Sm2—O13—C40 | -59.52 (17) |
| O11—Sm2—C40—O14 | -56.52 (17) | N3—Sm2—O13—C40 | 21.7 (2) |
| N3—Sm2—C40—O14 | 18.84 (18) | C48—Sm2—O13—C40 | 97.69 (17) |
| C48—Sm2—C40—O14 | 94.02 (17) | C32—Sm2—O13—C40 | -82.41 (17) |
| C32—Sm2—C40—O14 | -81.54 (17) | O13—C40—O14—Sm2 | -1.1 (3) |
| O8—Sm2—C40—O13 | 7.03 (17) | C39—C40—O14—Sm2 | 177.3 (2) |
| O14—Sm2—C40—O13 | 178.9 (3) | O8—Sm2—O14—C40 | 10.1 (2) |
| O2W—Sm2—C40—O13 | 95.9 (2) | O13—Sm2—O14—C40 | 0.64 (16) |
| O16—Sm2—C40—O13 | -80.64 (18) | O2W—Sm2—O14—C40 | 140.64 (16) |
| O17—Sm2—C40—O13 | -88.47 (17) | O16—Sm2—O14—C40 | -99.49 (17) |
| O10—Sm2—C40—O13 | 72.22 (16) | O17—Sm2—O14—C40 | -80.88 (17) |
| O11—Sm2—C40—O13 | 122.35 (17) | O10—Sm2—O14—C40 | 71.96 (17) |
| N3—Sm2—C40—O13 | -162.29 (16) | O11—Sm2—O14—C40 | 119.62 (17) |
| C48—Sm2—C40—O13 | -87.11 (17) | N3—Sm2—O14—C40 | -160.90 (18) |
| C32—Sm2—C40—O13 | 97.32 (17) | C48—Sm2—O14—C40 | -91.52 (17) |
| C46—C41—C42—C43 | 0.0 (4) | C32—Sm2—O14—C40 | 96.54 (17) |
| C47—C41—C42—C43 | 177.1 (3) | O17—C48—O16—Sm2 | 9.3 (3) |
| C41—C42—C43—C44 | -1.3 (5) | C47—C48—O16—Sm2 | -169.6 (2) |
| C42—C43—C44—O18 | -178.4 (3) | O8—Sm2—O16—C48 | -112.93 (16) |
| C42—C43—C44—C45 | 1.9 (5) | O14—Sm2—O16—C48 | 18.30 (19) |
| O18—C44—C45—C46 | 179.2 (3) | O13—Sm2—O16—C48 | -44.99 (17) |
| C43—C44—C45—C46 | -1.3 (5) | O2W—Sm2—O16—C48 | 166.54 (17) |
| C44—C45—C46—C41 | -0.1 (5) | O17—Sm2—O16—C48 | -5.15 (15) |
| C42—C41—C46—C45 | 0.7 (4) | O10—Sm2—O16—C48 | -147.80 (15) |
| C47—C41—C46—C45 | -176.5 (3) | O11—Sm2—O16—C48 | 127.73 (16) |
| C42—C41—C47—C48 | -69.6 (4) | N3—Sm2—O16—C48 | 79.21 (16) |
| C46—C41—C47—C48 | 107.4 (3) | C40—Sm2—O16—C48 | -14.81 (19) |

supplementary materials

| | | | |
|-----------------|--------------|-----------------|--------------|
| C41—C47—C48—O16 | 57.3 (4) | C32—Sm2—O16—C48 | 168.84 (15) |
| C41—C47—C48—O17 | -121.6 (3) | O16—C48—O17—Sm2 | -9.0 (3) |
| O8—Sm2—C48—O16 | 65.60 (16) | C47—C48—O17—Sm2 | 169.9 (2) |
| O14—Sm2—C48—O16 | -165.05 (15) | O8—Sm2—O17—C48 | 77.00 (17) |
| O13—Sm2—C48—O16 | 140.81 (15) | O14—Sm2—O17—C48 | -155.86 (17) |
| O2W—Sm2—C48—O16 | -13.28 (17) | O13—Sm2—O17—C48 | 149.37 (18) |
| O17—Sm2—C48—O16 | 170.8 (3) | O2W—Sm2—O17—C48 | -5.1 (2) |
| O10—Sm2—C48—O16 | 68.1 (3) | O16—Sm2—O17—C48 | 5.04 (15) |
| O11—Sm2—C48—O16 | -87.5 (2) | O10—Sm2—O17—C48 | 134.67 (16) |
| N3—Sm2—C48—O16 | -93.97 (16) | O11—Sm2—O17—C48 | -120.14 (17) |
| C40—Sm2—C48—O16 | 167.87 (16) | N3—Sm2—O17—C48 | -78.00 (17) |
| O8—Sm2—C48—O17 | -105.24 (17) | C40—Sm2—O17—C48 | 176.99 (18) |
| O14—Sm2—C48—O17 | 24.12 (17) | C32—Sm2—O17—C48 | -164.1 (2) |

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------------------|----------|-------------|-------------|---------------|
| O3—H3B \cdots O12 ⁱ | 0.82 | 1.94 | 2.749 (3) | 169 |
| O6—H6B \cdots O3W ⁱⁱ | 0.82 | 1.86 | 2.642 (3) | 159 |
| O9—H9A \cdots O17 ⁱⁱⁱ | 0.82 | 1.86 | 2.673 (3) | 173 |
| O12—H12A \cdots O11 ^{iv} | 0.82 | 1.94 | 2.746 (3) | 168 |
| O15—H15C \cdots O6 ^v | 0.82 | 1.91 | 2.722 (3) | 174 |
| O18—H18B \cdots O9 ⁱⁱ | 0.82 | 1.95 | 2.768 (3) | 173 |
| O2W—H2WA \cdots O5 | 0.83 (5) | 2.02 (5) | 2.767 (3) | 150 (4) |
| O2W—H2WB \cdots N2 ⁱⁱ | 0.83 (2) | 2.03 (2) | 2.841 (3) | 164 (5) |
| O3W—H3WB \cdots O3 | 0.85 (4) | 1.99 (2) | 2.816 (3) | 167 (5) |
| O1W—H1WA \cdots O13 | 0.81 (5) | 1.96 (4) | 2.755 (3) | 165 (4) |
| O1W—H1WB \cdots N4 ⁱ | 0.83 (2) | 1.99 (2) | 2.778 (3) | 160 (4) |
| O3W—H3WA \cdots O1 ^{vi} | 0.84 (4) | 1.94 (4) | 2.773 (3) | 172 (4) |

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

Fig. 1

