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Retraction of articles by T. Liu *et al.*

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A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *et al.* are retracted. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)	Liu & Xie (2007*a*)	10.1107/S1600536807026852	EDUMAS
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*b*)	10.1107/S1600536807028255	EDUVAB
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)	Liu & Xie (2007*b*)	10.1107/S1600536807028735	RIGQAA
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]	Liu, Wang, Wang & Xie (2007*c*)	10.1107/S1600536807030917	UDUMIQ
Polymeric $KNOF_2$	Liu Wang, Wang & Xie (2007*a*)	10.1107/S1600536807027195	ICSD 240891
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')cobalt(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*d*)	10.1107/S1600536807031224	WIHJED
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]	Liu, Wang, Wang & Xie (2007*e*)	10.1107/S1600536807032679	WIHQEK
Tetrakis[μ-(2-pyridyloxy)acetato-$\kappa^2O:O'$]bis{(1,10-phenanthroline-κ^2N,N')-[(2-pyridyloxy)acetato-κO]neodymium(III)}	Liu, Wang, Wang & Xie (2007*f*)	10.1107/S1600536807035349	TIGDAP
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')manganese(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*g*)	10.1107/S1600536807035076	TIGDET
2-Amino-3,5-dinitrobenzoic acid–ammonia (1/1)	Liu & Zhu (2007*j*)	10.1107/S1600536807040068	KIKQAX
2-Hydroxy-3,5-dinitrobenzamide monohydrate	Liu & Zhu (2007*k*)	10.1107/S1600536807039712	KIKQEB
2-(1-Hydroxy-2-pyridyl)acetamide monohydrate	Liu & Zhu (2007*l*)	10.1107/S1600536807040652	CIKQOD
Bis(2,2′-bipyridine-κN,N′)bis(thiocyanato-κN)iron(II)	Liu & Zhu (2007*a*)	10.1107/S1600536807043486	XIFXOA
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III]	Liu & Zhu (2007*b*)	10.1107/S1600536807045485	XILNAI
3-Hydroxy-2,4,6-trinitropyridine monohydrate	Liu & Zhu (2007*m*)	10.1107/S1600536807045230	PILNOO
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]	Liu & Zhu (2007*c*)	10.1107/S1600536807047733	SILZET
catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]	Liu & Zhu (2007*d*)	10.1107/S1600536807050969	GIMZOS
Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)	Liu & Zhu (2007*e*)	10.1107/S1600536807051756	WINFAB
2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate	Liu & Zhu (2007*n*)	10.1107/S1600536807048477	GINFEP
2-(Benzoylhydrazinocarbonyl)benzoic acid	Liu & Zhu (2007*o*)	10.1107/S160053680705204X	TINZIA
Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)	Liu & Zhu (2007*f*)	10.1107/S1600536807054529	HIPZIQ
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*g*)	10.1107/S1600536807056504	XIRGIP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*h*)	10.1107/S1600536807059077	HIQROP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetamidato-$\kappa^2O:N$]	Liu & Zhu (2007*i*)	10.1107/S1600536807060631	YIQMER
N′-Benzoyl-4-nitronicotinohydrazide	Liu & Zhu (2007*p*)	10.1107/S1600536807053068	CIPVON
N′-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide	Liu & Zhu (2007*q*)	10.1107/S1600536807054876	RIRWEV

 doi:10.1107/S1600536809049976

Table 1 (continued)

Title	Reference	DOI	Refcode
Ethylenediammonium sulfate	Liu & Zhu (2007*r*)	10.1107/S1600536807056280	ETDAMS03
Ethylenediammonium perchlorate	Liu & Zhu (2007*s*)	10.1107/S1600536807059909	HIRYEN
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')manganese(II)]-μ-nitrato-$\kappa^2O:O'$]	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

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Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007*d*). *Acta Cryst.* E**63**, m2027–m2028.
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007*e*). *Acta Cryst.* E**63**, m2080–m2081.
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007*f*). *Acta Cryst.* E**63**, m2196–m2197.
Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007*g*). *Acta Cryst.* E**63**, m2198–m2199.
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Liu, T. & Zhu, J. Y. (2007*h*). *Acta Cryst.* E**63**, m3108.
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catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III)]

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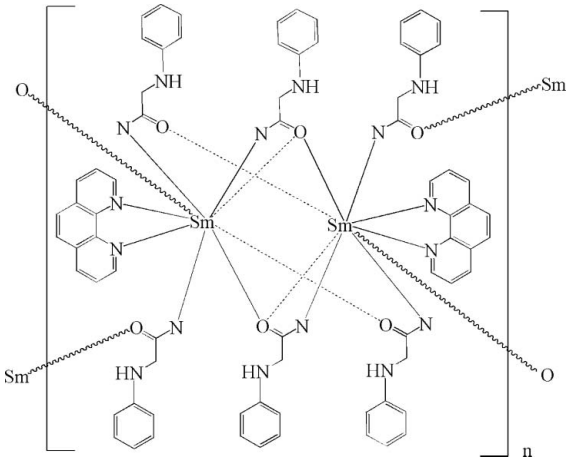
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.013 Å; R factor = 0.051; wR factor = 0.160; data-to-parameter ratio = 17.8.

The molecule of the title compound, $[Sm_2(C_8H_9N_2O)_6(C_{12}H_8N_2)_2]_n$, is a binuclear polymeric complex and has an inversion centre midway between the two Sm^{III} ions, which are bridged by two tridentate, two bidentate and four mondentate (within the binuclear unit) acetamide groups. Each Sm atom is nine-coordinated by two N atoms of a 1,10-phenanthroline ligand and four O and three N atoms of anilinoacetamide ligands. In the crystal structure, intermolecular C—H···O, C—H···N, N—H···O and N—H···N hydrogen bonds result in the formation of a supramolecular network structure; an intramolecular N—H···O hydrogen bond is also present.

Related literature

For related literature, see: Daiguebonne *et al.* (2000); Farrugia *et al.* (2000); Tsukube & Shinoda (2002); Zhang *et al.* (2005); Starynowicz (1991); Starynowicz (1993); Kay *et al.* (1972); Ma *et al.* (1999); Zeng *et al.* (2000); Mao *et al.* (1998). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{36}H_{35}N_8O_3Sm$
M_r = 778.08
Monoclinic, $P2_1/n$
a = 19.876 (3) Å
b = 8.5511 (17) Å
c = 20.481 (4) Å
β = 106.871 (9)°
V = 3331.2 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.81 mm^{-1}
T = 273 (2) K
0.33 × 0.12 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.587, T_{max} = 0.870
26612 measured reflections
7330 independent reflections
4913 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.160
S = 1.04
7330 reflections
411 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sm1—O1	2.561 (4)	Sm1—N7	2.448 (4)
Sm1—O2^{i}	2.505 (4)	Sm1—N8	2.418 (4)
Sm1—O3^{ii}	2.535 (4)	Sm1—N9^{i}	2.404 (4)
Sm1—N1	2.713 (5)	Sm1—N9	2.846 (5)
Sm1—N2	2.685 (5)		
O1—Sm1—N1	63.78 (13)	N1—Sm1—N9	102.57 (14)
O1—Sm1—N2	74.82 (13)	N2—Sm1—N7	81.57 (14)
O1—Sm1—N7	73.24 (13)	N2—Sm1—N8	95.78 (14)
O1—Sm1—N8	139.47 (13)	N2—Sm1—N9	118.50 (12)
O1—Sm1—N9	47.76 (11)	N7—Sm1—N8	145.52 (14)
N1—Sm1—N2	59.51 (15)	N7—Sm1—N9	64.51 (12)
N1—Sm1—N7	127.34 (13)	N8—Sm1—N9	140.58 (12)
N1—Sm1—N8	77.35 (14)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O2^{i}	0.93	2.41	3.100 (8)	131
C10—H10···O1^{iii}	0.93	2.32	3.188 (8)	155
C12—H12···O3^{ii}	0.93	2.45	3.039 (8)	121
C12—H12···N5^{ii}	0.93	2.54	3.387 (9)	151
C22—H22B···N8^{iv}	0.97	2.37	3.310 (8)	162
N9—H9···O2^{i}	0.86	2.14	2.889 (6)	146
N9—H9···N9^{i}	0.86	2.61	3.136 (9)	120
N8—H8···O2^{i}	0.79 (2)	2.31 (3)	3.062 (6)	160 (6)
N3—H3A···O2	0.86	2.24	2.595 (5)	105

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2324).

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supplementary materials

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catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III]

T. Liu and J.-Y. Zhu

Comment

In recent years, there has been great interest in the synthesis of metal organic frameworks (MOFs) with organic ligands and rare earth metals because of their novel structures, fascinating properties and important roles in special materials having optical, electronic, magnetic and biological importance potential applications (Daiguebonne *et al.*, 2000; Farrugia *et al.*, 2000; Tsukube & Shinoda, 2002; Zhang *et al.*, 2005). These compounds are usually prepared by the reaction of rare-earth metal ions with bi- or multidentate ligands (Starynowicz, 1991, 1993; Kay *et al.*, 1972; Ma *et al.*, 1999; Zeng *et al.*, 2000; Mao *et al.*, 1998). We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). It has an inversion centre midway between the two Sm^{III} ions, which are bridged by two terdentate, two bidentate and four monodentate acetamide groups. Each Sm atom is nine-coordinated by two N atoms of a 1,10-phenanthroline (phen) ligand and four O and three N atoms of anilinoacetamide ligands. The Sm—O and Sm—N bonds are in the range of [2.505 (4)–2.561 (4) Å] and [2.404 (4)–2.846 (5) Å], respectively (Table 1).

In the crystal structure, intermolecular C—H···O, C—H···N, N—H···O and N–H···N hydrogen bonds (Table 1, Fig. 2) result in the formation of a supramolecular network structure; intramolecular N—H···O hydrogen bond (Table 1) is also present.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Samarium (III) nitrate hexahydrate (218.5 mg, 0.5 mmol), phen (198 mg, 1 mmol), anilinoacetamide (145.2 mg, 1 mmol) and distilled water (6 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 423 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H5 and H8 (for NH) were located in difference syntheses and refined isotropically [N—H = 0.84 (5) and 0.79 (2) Å, U_{iso}(H) = 0.08 (2) and 0.077 (19) $Å^2$]. The remaining H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93 and 0.97 Å, for aromatic and methylene H atoms and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

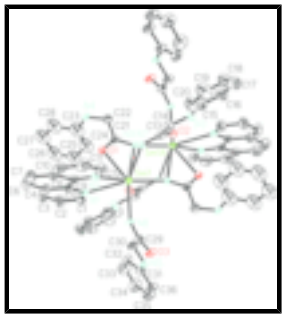


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): 2 − *x*, −*y*, 2 − *z*]. H atoms have been omitted for clarity.

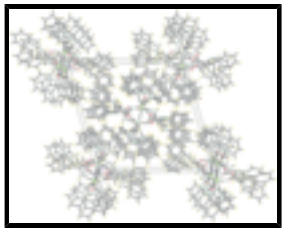


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

catena-Poly[hexakis(μ$_2$-anilinoacetamide)bis(1,10- phenanthroline)disamarium(III]

Crystal data

$C_{36}H_{35}N_8O_3Sm$	F_{000} = 1572
M_r = 778.08	D_x = 1.551 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: -P 2yn	λ = 0.71073 Å
a = 19.876 (3) Å	Cell parameters from 8983 reflections
b = 8.5511 (17) Å	θ = 2.6–26.7º
c = 20.481 (4) Å	μ = 1.81 mm^{-1}
β = 106.871 (9)º	T = 273 (2) K
V = 3331.2 (11) Å^3	Plate, colourless
Z = 4	0.33 × 0.12 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer	7330 independent reflections
Radiation source: fine-focus sealed tube	4913 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 273(2) K	θ_{max} = 27.3º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→25
T_{min} = 0.587, T_{max} = 0.870	k = −10→11
26612 measured reflections	l = −26→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.160$	$w = 1/[\sigma^2(F_o^2) + (0.1002P)^2 + 0.285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
7330 reflections	$\Delta\rho_{max} = 1.58$ e Å^{-3}
411 parameters	$\Delta\rho_{min} = -0.90$ e Å^{-3}
7 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sm1	0.931195 (14)	0.19069 (3)	0.964291 (13)	0.03946 (13)
O1	0.84613 (18)	−0.0358 (4)	0.91906 (18)	0.0411 (8)
O2	1.0667 (2)	−0.0828 (5)	0.92142 (18)	0.0460 (9)
O3	1.0067 (2)	0.6126 (5)	1.09069 (18)	0.0526 (11)
N1	0.7967 (2)	0.2337 (6)	0.9666 (2)	0.0438 (11)
N2	0.8343 (3)	0.3064 (5)	0.8548 (2)	0.0446 (11)
N3	1.1178 (2)	−0.0165 (6)	0.8216 (2)	0.0478 (12)
H3A	1.1392	−0.0748	0.8555	0.057*
N4	0.7856 (2)	−0.3269 (5)	0.8983 (3)	0.0437 (11)
H4	0.7623	−0.3415	0.8562	0.052*
N5	0.9876 (3)	0.5266 (6)	1.2064 (2)	0.0422 (11)
H5	0.960 (3)	0.602 (5)	1.205 (2)	0.08 (2)*
N7	0.9710 (2)	0.0616 (5)	0.87541 (18)	0.0295 (8)
H7A	0.9397	0.0561	0.8363	0.035*
N8	0.9399 (2)	0.4227 (5)	1.03379 (19)	0.0300 (8)
H8	0.938 (3)	0.331 (2)	1.036 (3)	0.077 (19)*

N9	0.9473 (2)	−0.1396 (5)	0.9772 (2)	0.0321 (9)
H9	0.9443	−0.0481	0.9935	0.038*
C1	0.7786 (4)	0.1912 (8)	1.0196 (4)	0.0610 (18)
H1	0.8137	0.1678	1.0596	0.073*
C2	0.7091 (4)	0.1790 (10)	1.0192 (5)	0.079 (2)
H2	0.6977	0.1495	1.0584	0.095*
C3	0.6583 (4)	0.2104 (10)	0.9615 (6)	0.087 (3)
H3	0.6114	0.1993	0.9603	0.104*
C4	0.6742 (4)	0.2576 (11)	0.9055 (4)	0.072 (2)
C5	0.7467 (3)	0.2676 (7)	0.9096 (3)	0.0496 (15)
C6	0.6215 (5)	0.2949 (13)	0.8391 (6)	0.109 (4)
H6	0.5738	0.2842	0.8346	0.110*
C7	0.6416 (5)	0.3424 (12)	0.7873 (5)	0.096 (3)
H7	0.6078	0.3696	0.7470	0.086*
C8	0.7132 (4)	0.3536 (9)	0.7907 (3)	0.0649 (19)
C9	0.7667 (3)	0.3093 (6)	0.8507 (3)	0.0497 (15)
C10	0.7357 (6)	0.4045 (10)	0.7375 (4)	0.086 (3)
H10	0.7032	0.4403	0.6979	0.083*
C11	0.8048 (5)	0.4033 (10)	0.7419 (3)	0.078 (2)
H11	0.8199	0.4381	0.7055	0.083*
C12	0.8528 (4)	0.3503 (8)	0.8008 (3)	0.0610 (17)
H12	0.9000	0.3453	0.8024	0.073*
C13	1.0285 (3)	0.0027 (7)	0.8772 (3)	0.0426 (13)
C14	1.0522 (3)	0.0523 (8)	0.8174 (3)	0.0514 (15)
H14A	1.0178	0.0204	0.7754	0.062*
H14B	1.0564	0.1653	0.8170	0.062*
C15	1.1460 (4)	0.0136 (8)	0.7692 (3)	0.0603 (17)
C16	1.2072 (4)	−0.0568 (10)	0.7758 (4)	0.073 (2)
H16	1.2275	−0.1199	0.8134	0.088*
C17	1.2396 (5)	−0.0342 (11)	0.7260 (6)	0.089 (3)
H17	1.2833	−0.0793	0.7304	0.087*
C18	1.2085 (6)	0.0534 (11)	0.6703 (6)	0.104 (3)
H18	1.2304	0.0643	0.6361	0.104*
C19	1.1479 (6)	0.1235 (13)	0.6637 (5)	0.107 (3)
H19	1.1273	0.1843	0.6255	0.108*
C20	1.1144 (5)	0.1048 (10)	0.7156 (4)	0.079 (2)
H20	1.0720	0.1540	0.7127	0.094*
C21	0.8831 (3)	−0.1522 (7)	0.9385 (3)	0.0424 (13)
C22	0.8576 (3)	−0.3143 (7)	0.9200 (3)	0.0527 (15)
H22A	0.8764	−0.3516	0.8840	0.063*
H22B	0.8757	−0.3815	0.9593	0.063*
C23	0.7552 (8)	−0.3148 (11)	0.9473 (8)	0.1209 (19)
C24	0.7842 (8)	−0.2800 (11)	1.0107 (8)	0.1209 (19)
H24	0.8323	−0.2617	1.0267	0.124*
C25	0.7417 (7)	−0.2701 (12)	1.0557 (7)	0.1209 (19)
H25	0.7616	−0.2473	1.1017	0.071*
C26	0.6749 (7)	−0.2935 (11)	1.0311 (8)	0.1209 (19)
H26	0.6478	−0.2824	1.0611	0.125*
C27	0.6373 (7)	−0.3361 (12)	0.9600 (7)	0.1209 (19)

H27	0.5894	−0.3571	0.9448	0.125*
C28	0.6791 (7)	−0.3412 (12)	0.9203 (7)	0.1209 (19)
H28	0.6599	−0.3621	0.8741	0.105*
C29	0.9693 (3)	0.4999 (7)	1.0864 (3)	0.0417 (12)
C30	0.9488 (4)	0.4461 (8)	1.1474 (3)	0.0525 (15)
H30A	0.8990	0.4644	1.1400	0.063*
H30B	0.9573	0.3347	1.1537	0.063*
C31	0.9740 (3)	0.4892 (8)	1.2654 (3)	0.0529 (15)
C32	0.9277 (4)	0.3786 (10)	1.2720 (3)	0.0670 (19)
H32	0.9021	0.3227	1.2340	0.080*
C33	0.9188 (6)	0.3494 (14)	1.3336 (5)	0.104 (3)
H33	0.8876	0.2721	1.3384	0.105*
C34	0.9568 (5)	0.4361 (13)	1.3906 (4)	0.098 (3)
H34	0.9491	0.4208	1.4328	0.117*
C35	1.0044 (5)	0.5416 (11)	1.3836 (4)	0.085 (2)
H35	1.0310	0.5959	1.4217	0.082*
C36	1.0144 (4)	0.5700 (9)	1.3221 (3)	0.0682 (19)
H36	1.0478	0.6424	1.3179	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.04558 (19)	0.0348 (2)	0.03320 (18)	−0.00143 (12)	0.00387 (12)	0.00068 (11)
O1	0.0412 (19)	0.032 (2)	0.042 (2)	0.0004 (17)	0.0003 (16)	−0.0024 (16)
O2	0.056 (2)	0.045 (2)	0.037 (2)	0.0067 (19)	0.0140 (17)	0.0098 (18)
O3	0.077 (3)	0.049 (3)	0.033 (2)	−0.024 (2)	0.0180 (19)	−0.0050 (18)
N1	0.041 (3)	0.041 (3)	0.043 (3)	0.003 (2)	0.002 (2)	−0.008 (2)
N2	0.055 (3)	0.040 (3)	0.030 (2)	0.003 (2)	−0.001 (2)	0.0008 (19)
N3	0.048 (3)	0.063 (3)	0.038 (2)	0.016 (2)	0.022 (2)	0.021 (2)
N4	0.040 (2)	0.033 (3)	0.049 (3)	−0.0123 (19)	−0.002 (2)	−0.006 (2)
N5	0.060 (3)	0.041 (3)	0.026 (2)	−0.020 (3)	0.015 (2)	−0.0051 (18)
N7	0.034 (2)	0.033 (2)	0.0202 (18)	0.0040 (18)	0.0060 (15)	0.0010 (16)
N8	0.048 (2)	0.015 (2)	0.026 (2)	−0.0049 (18)	0.0083 (17)	−0.0041 (16)
N9	0.033 (2)	0.026 (2)	0.030 (2)	−0.0012 (17)	−0.0016 (16)	0.0041 (16)
C1	0.054 (4)	0.073 (5)	0.056 (4)	0.007 (3)	0.016 (3)	−0.001 (3)
C2	0.055 (4)	0.110 (7)	0.077 (5)	0.004 (4)	0.027 (4)	−0.010 (5)
C3	0.045 (4)	0.096 (7)	0.116 (8)	−0.005 (4)	0.020 (5)	−0.014 (6)
C4	0.051 (4)	0.086 (5)	0.067 (5)	0.006 (4)	−0.002 (4)	−0.015 (4)
C5	0.050 (3)	0.034 (3)	0.056 (4)	0.008 (3)	0.002 (3)	−0.008 (3)
C6	0.052 (5)	0.140 (11)	0.105 (8)	0.016 (5)	−0.023 (5)	−0.036 (7)
C7	0.081 (6)	0.107 (7)	0.070 (6)	0.037 (5)	−0.026 (5)	−0.012 (5)
C8	0.067 (4)	0.064 (4)	0.042 (4)	0.019 (4)	−0.017 (3)	−0.011 (3)
C9	0.058 (4)	0.032 (3)	0.045 (3)	0.005 (3)	−0.007 (3)	−0.004 (2)
C10	0.121 (7)	0.064 (5)	0.043 (4)	0.016 (5)	−0.022 (4)	0.000 (3)
C11	0.112 (7)	0.078 (6)	0.030 (3)	−0.002 (5)	0.000 (4)	0.013 (3)
C12	0.076 (5)	0.051 (4)	0.047 (4)	−0.001 (3)	0.004 (3)	0.009 (3)
C13	0.059 (3)	0.034 (3)	0.033 (3)	−0.013 (3)	0.010 (2)	−0.004 (2)
C14	0.060 (4)	0.053 (4)	0.043 (3)	0.006 (3)	0.017 (3)	0.010 (3)

C15	0.066 (4)	0.068 (5)	0.053 (4)	−0.012 (4)	0.028 (3)	0.001 (3)
C16	0.072 (5)	0.093 (6)	0.065 (4)	0.006 (4)	0.036 (4)	−0.001 (4)
C17	0.081 (6)	0.094 (7)	0.108 (7)	−0.004 (5)	0.052 (5)	−0.010 (6)
C18	0.140 (9)	0.077 (6)	0.135 (9)	−0.014 (6)	0.104 (8)	0.000 (6)
C19	0.152 (10)	0.108 (7)	0.086 (7)	0.020 (7)	0.076 (7)	0.034 (6)
C20	0.093 (6)	0.087 (6)	0.072 (5)	0.002 (5)	0.050 (5)	0.020 (4)
C21	0.044 (3)	0.050 (4)	0.028 (3)	−0.005 (3)	0.003 (2)	−0.005 (2)
C22	0.058 (4)	0.047 (4)	0.048 (4)	0.001 (3)	0.008 (3)	−0.007 (3)
C23	0.133 (4)	0.090 (3)	0.162 (5)	0.016 (3)	0.078 (4)	0.031 (3)
C24	0.133 (4)	0.090 (3)	0.162 (5)	0.016 (3)	0.078 (4)	0.031 (3)
C25	0.133 (4)	0.090 (3)	0.162 (5)	0.016 (3)	0.078 (4)	0.031 (3)
C26	0.133 (4)	0.090 (3)	0.162 (5)	0.016 (3)	0.078 (4)	0.031 (3)
C27	0.133 (4)	0.090 (3)	0.162 (5)	0.016 (3)	0.078 (4)	0.031 (3)
C28	0.133 (4)	0.090 (3)	0.162 (5)	0.016 (3)	0.078 (4)	0.031 (3)
C29	0.054 (3)	0.031 (3)	0.039 (3)	−0.001 (3)	0.013 (2)	0.005 (2)
C30	0.071 (4)	0.050 (4)	0.037 (3)	−0.021 (3)	0.016 (3)	−0.005 (3)
C31	0.071 (4)	0.054 (4)	0.032 (3)	−0.004 (3)	0.013 (3)	0.003 (3)
C32	0.068 (4)	0.089 (5)	0.044 (4)	−0.032 (4)	0.017 (3)	−0.005 (3)
C33	0.119 (8)	0.136 (8)	0.071 (6)	−0.045 (7)	0.049 (6)	0.004 (6)
C34	0.114 (7)	0.141 (9)	0.045 (4)	−0.028 (7)	0.033 (4)	0.005 (5)
C35	0.111 (6)	0.098 (6)	0.041 (4)	−0.019 (5)	0.013 (4)	−0.009 (4)
C36	0.079 (5)	0.075 (5)	0.047 (4)	−0.018 (4)	0.012 (3)	−0.012 (3)

Geometric parameters (Å, °)

Sm1—O1	2.561 (4)	C8—C9	1.424 (8)
Sm1—O2^{i}	2.505 (4)	C10—C11	1.350 (12)
Sm1—O3^{ii}	2.535 (4)	C10—H10	0.9300
Sm1—N1	2.713 (5)	C11—C12	1.380 (9)
Sm1—N2	2.685 (5)	C11—H11	0.9300
Sm1—N7	2.448 (4)	C12—H12	0.9300
Sm1—N8	2.418 (4)	C13—C14	1.494 (8)
Sm1—N9^{i}	2.404 (4)	C14—H14A	0.9700
Sm1—N9	2.846 (5)	C14—H14B	0.9700
O1—C21	1.233 (7)	C15—C16	1.328 (10)
O2—C13	1.238 (6)	C15—C20	1.343 (10)
O2—Sm1^{i}	2.505 (4)	C16—C17	1.370 (11)
O3—C29	1.205 (7)	C16—H16	0.9300
O3—Sm1^{ii}	2.535 (4)	C17—C18	1.355 (13)
N1—C1	1.291 (8)	C17—H17	0.9300
N1—C5	1.327 (7)	C18—C19	1.317 (13)
N2—C12	1.318 (8)	C18—H18	0.9300
N2—C9	1.321 (8)	C19—C20	1.417 (10)
N3—C15	1.373 (7)	C19—H19	0.9300
N3—C14	1.410 (7)	C20—H20	0.9300
N3—H3A	0.8600	C21—C22	1.488 (8)
N4—C23	1.317 (14)	C22—H22A	0.9700
N4—C22	1.374 (8)	C22—H22B	0.9700

N4—H4	0.8600	C23—C24	1.295 (19)
N5—C31	1.351 (7)	C23—C28	1.468 (18)
N5—C30	1.410 (7)	C24—C25	1.421 (15)
N5—H5	0.84 (5)	C24—H24	0.9300
N7—C13	1.241 (7)	C25—C26	1.293 (17)
N7—H7A	0.8600	C25—H25	0.9300
N8—C29	1.254 (7)	C26—C27	1.476 (18)
N8—H8	0.79 (2)	C26—H26	0.9300
N9—C21	1.295 (7)	C27—C28	1.322 (14)
N9—Sm1^{i}	2.404 (4)	C27—H27	0.9300
N9—H9	0.8600	C28—H28	0.9300
C1—C2	1.384 (10)	C29—C30	1.495 (8)
C1—H1	0.9300	C30—H30A	0.9700
C2—C3	1.340 (12)	C30—H30B	0.9700
C2—H2	0.9300	C31—C32	1.353 (9)
C3—C4	1.338 (12)	C31—C36	1.389 (9)
C3—H3	0.9300	C32—C33	1.349 (10)
C4—C5	1.420 (10)	C32—H32	0.9300
C4—C6	1.490 (12)	C33—C34	1.404 (13)
C5—C9	1.421 (9)	C33—H33	0.9300
C6—C7	1.303 (15)	C34—C35	1.346 (12)
C6—H6	0.9300	C34—H34	0.9300
C7—C8	1.407 (13)	C35—C36	1.351 (10)
C7—H7	0.9300	C35—H35	0.9300
C8—C10	1.362 (12)	C36—H36	0.9300
O1—Sm1—N1	63.78 (13)	N1—C5—C9	118.6 (6)
O1—Sm1—N2	74.82 (13)	C4—C5—C9	119.6 (6)
O1—Sm1—N7	73.24 (13)	C7—C6—C4	120.6 (9)
O1—Sm1—N8	139.47 (13)	C7—C6—H6	119.7
O1—Sm1—N9	47.76 (11)	C4—C6—H6	119.7
N1—Sm1—N2	59.51 (15)	C6—C7—C8	121.7 (8)
N1—Sm1—N7	127.34 (13)	C6—C7—H7	119.1
N1—Sm1—N8	77.35 (14)	C8—C7—H7	119.1
N1—Sm1—N9	102.57 (14)	C10—C8—C7	122.9 (7)
N2—Sm1—N7	81.57 (14)	C10—C8—C9	116.0 (7)
N2—Sm1—N8	95.78 (14)	C7—C8—C9	121.1 (8)
N2—Sm1—N9	118.50 (12)	N2—C9—C5	118.1 (5)
N7—Sm1—N8	145.52 (14)	N2—C9—C8	123.5 (6)
N7—Sm1—N9	64.51 (12)	C5—C9—C8	118.4 (6)
N8—Sm1—N9	140.58 (12)	C11—C10—C8	120.5 (7)
N9^{i}—Sm1—N8	88.03 (15)	C11—C10—H10	119.7
N9^{i}—Sm1—N7	78.13 (13)	C8—C10—H10	119.7
N9^{i}—Sm1—O2^{i}	74.09 (13)	C10—C11—C12	119.5 (7)
N8—Sm1—O2^{i}	76.88 (13)	C10—C11—H11	120.2
N7—Sm1—O2^{i}	127.41 (13)	C12—C11—H11	120.2
N9^{i}—Sm1—O2^{i}	74.09 (13)	N2—C12—C11	122.5 (7)
N8—Sm1—O2^{i}	76.88 (13)	N2—C12—H12	118.8

N7—Sm1—O2^{i}	127.41 (13)	C11—C12—H12	118.8
O2^{i}—Sm1—O2^{i}	0.0 (3)	O2—C13—N7	128.7 (5)
N9^{i}—Sm1—O2^{i}	74.09 (13)	O2—C13—C14	119.6 (5)
N8—Sm1—O2^{i}	76.88 (13)	N7—C13—C14	111.6 (5)
N7—Sm1—O2^{i}	127.41 (13)	N3—C14—C13	109.7 (5)
O2^{i}—Sm1—O2^{i}	0.0 (3)	N3—C14—H14A	109.7
O2^{i}—Sm1—O2^{i}	0.0 (3)	C13—C14—H14A	109.7
N9^{i}—Sm1—O3^{ii}	78.11 (14)	N3—C14—H14B	109.7
N8—Sm1—O3^{ii}	75.89 (13)	C13—C14—H14B	109.7
N7—Sm1—O3^{ii}	70.44 (13)	H14A—C14—H14B	108.2
O2^{i}—Sm1—O3^{ii}	141.38 (13)	C16—C15—C20	123.0 (7)
O2^{i}—Sm1—O3^{ii}	141.38 (13)	C16—C15—N3	113.8 (6)
O2^{i}—Sm1—O3^{ii}	141.38 (13)	C20—C15—N3	123.2 (6)
N9^{i}—Sm1—O1	120.36 (14)	C15—C16—C17	118.3 (8)
O2^{i}—Sm1—O1	83.67 (12)	C15—C16—H16	120.9
O2^{i}—Sm1—O1	83.67 (12)	C17—C16—H16	120.9
O2^{i}—Sm1—O1	83.67 (12)	C18—C17—C16	120.5 (9)
O3^{ii}—Sm1—O1	134.14 (12)	C18—C17—H17	119.8
N9^{i}—Sm1—N2	148.94 (15)	C16—C17—H17	119.8
O2^{i}—Sm1—N2	136.81 (14)	C19—C18—C17	121.2 (8)
O2^{i}—Sm1—N2	136.81 (14)	C19—C18—H18	119.4
O2^{i}—Sm1—N2	136.81 (14)	C17—C18—H18	119.4
O3^{ii}—Sm1—N2	73.04 (15)	C18—C19—C20	119.1 (9)
N9^{i}—Sm1—N1	150.30 (14)	C18—C19—H19	120.5
O2^{i}—Sm1—N1	77.45 (14)	C20—C19—H19	120.5
O2^{i}—Sm1—N1	77.45 (14)	C15—C20—C19	117.9 (8)
O2^{i}—Sm1—N1	77.45 (14)	C15—C20—H20	121.0
O3^{ii}—Sm1—N1	121.79 (15)	C19—C20—H20	121.0
N9^{i}—Sm1—N9	72.79 (15)	O1—C21—N9	121.3 (5)
O2^{i}—Sm1—N9	64.97 (12)	O1—C21—C22	122.9 (5)
O2^{i}—Sm1—N9	64.97 (12)	N9—C21—C22	115.8 (5)
O2^{i}—Sm1—N9	64.97 (12)	N4—C22—C21	113.7 (5)
O3^{ii}—Sm1—N9	130.08 (13)	N4—C22—H22A	108.8
N9^{i}—Sm1—H8	84 (2)	C21—C22—H22A	108.8
N7—Sm1—H8	155.0 (19)	N4—C22—H22B	108.8
O2^{i}—Sm1—H8	61.7 (13)	C21—C22—H22B	108.8
O2^{i}—Sm1—H8	61.7 (13)	H22A—C22—H22B	107.7
O2^{i}—Sm1—H8	61.7 (13)	C24—C23—N4	127.9 (14)
O3^{ii}—Sm1—H8	89.2 (15)	C24—C23—C28	121.5 (13)
O1—Sm1—H8	131.4 (17)	N4—C23—C28	110.6 (13)
N2—Sm1—H8	106.9 (17)	C23—C24—C25	119.3 (15)

N1—Sm1—H8	75 (2)	C23—C24—H24	120.4
N9—Sm1—H8	125.7 (13)	C25—C24—H24	120.4
C21—O1—Sm1	103.0 (3)	C26—C25—C24	118.3 (15)
C13—O2—Sm1^{i}	137.9 (4)	C26—C25—H25	120.8
C29—O3—Sm1^{ii}	150.2 (4)	C24—C25—H25	120.8
C1—N1—C5	118.8 (6)	C25—C26—C27	126.2 (13)
C1—N1—Sm1	119.5 (4)	C25—C26—H26	116.9
C5—N1—Sm1	120.3 (4)	C27—C26—H26	116.9
C12—N2—C9	117.8 (5)	C28—C27—C26	112.7 (13)
C12—N2—Sm1	119.9 (4)	C28—C27—H27	123.6
C9—N2—Sm1	122.0 (4)	C26—C27—H27	123.6
C15—N3—C14	117.1 (5)	C27—C28—C23	121.8 (15)
C15—N3—H3A	121.5	C27—C28—H28	119.1
C14—N3—H3A	121.5	C23—C28—H28	119.1
C23—N4—C22	114.4 (9)	O3—C29—N8	127.4 (5)
C23—N4—H4	122.8	O3—C29—C30	119.9 (5)
C22—N4—H4	122.8	N8—C29—C30	112.6 (5)
C31—N5—C30	116.7 (5)	N5—C30—C29	110.6 (5)
C31—N5—H5	85.3 (17)	N5—C30—H30A	109.5
C30—N5—H5	99 (5)	C29—C30—H30A	109.5
C13—N7—Sm1	131.0 (3)	N5—C30—H30B	109.5
C13—N7—H7A	114.5	C29—C30—H30B	109.5
Sm1—N7—H7A	114.5	H30A—C30—H30B	108.1
C29—N8—Sm1	150.9 (4)	N5—C31—C32	124.9 (6)
C29—N8—H8	120 (5)	N5—C31—C36	114.4 (6)
C21—N9—Sm1^{i}	163.3 (4)	C32—C31—C36	120.6 (6)
C21—N9—Sm1	87.8 (3)	C32—C31—H5	124 (3)
Sm1^{i}—N9—Sm1	107.21 (15)	C36—C31—H5	107 (3)
C21—N9—H9	98.3	C33—C32—C31	120.1 (7)
Sm1^{i}—N9—H9	98.3	C33—C32—H32	120.0
N1—C1—C2	122.5 (7)	C31—C32—H32	120.0
N1—C1—H1	118.8	C32—C33—C34	119.7 (8)
C2—C1—H1	118.8	C32—C33—H33	120.2
C3—C2—C1	119.0 (8)	C34—C33—H33	120.2
C3—C2—H2	120.5	C35—C34—C33	119.4 (7)
C1—C2—H2	120.5	C35—C34—H34	120.3
C4—C3—C2	120.8 (8)	C33—C34—H34	120.3
C4—C3—H3	119.6	C34—C35—C36	121.2 (7)
C2—C3—H3	119.6	C34—C35—H35	119.4
C3—C4—C5	117.1 (7)	C36—C35—H35	119.4
C3—C4—C6	124.6 (8)	C35—C36—C31	118.9 (7)
C5—C4—C6	118.3 (8)	C35—C36—H36	120.5
N1—C5—C4	121.8 (6)	C31—C36—H36	120.5

Symmetry codes: (i) −*x*+2, −*y*, −*z*+2; (ii) −*x*+2, −*y*+1, −*z*+2.

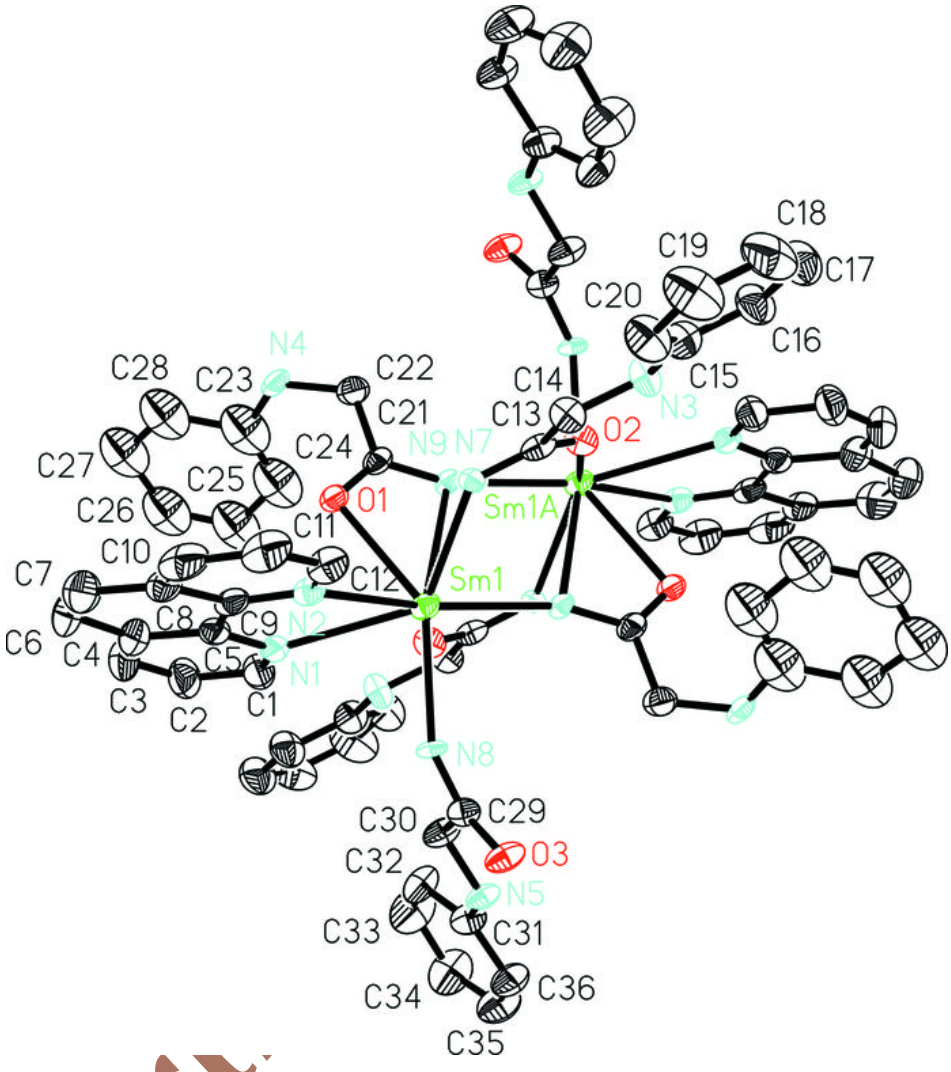
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

C1—H1···O2^{i}	0.93	2.41	3.100 (8)	131
C10—H10···O1^{iii}	0.93	2.32	3.188 (8)	155
C12—H12···O3^{ii}	0.93	2.45	3.039 (8)	121
C12—H12···N5^{ii}	0.93	2.54	3.387 (9)	151
C22—H22B···N8^{iv}	0.97	2.37	3.310 (8)	162
N9—H9···O2^{i}	0.86	2.14	2.889 (6)	146
N9—H9···N9^{i}	0.86	2.61	3.136 (9)	120
N8—H8···O2^{i}	0.79 (2)	2.31 (3)	3.062 (6)	160 (6)
N3—H3A···O2	0.86	2.24	2.595 (5)	105

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

Fig. 1


C18
C19
C17
C20
C16
C15
N4
C28
C23
C22
C14
N3
C21
C13
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C24
N9
N7
C27
C25
O1
Sm1A
C26
C11
C10
C7
C12
Sm1
C8
C9
N2
C6
C4
C5
N1
C3
C2
C1
N8
C30
C29
O3
C32
N5
C33
C31
C34
C36
C35

Fig. 2