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Tetrakis(μ-naphthalene-1-acetato)bis[(naphthalene-1-acetato)(1,10-phenanthroline)ytterbium(III)]

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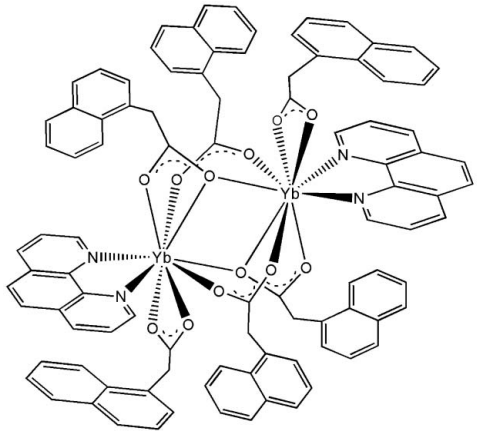
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.031; wR factor = 0.089; data-to-parameter ratio = 12.9.

The title complex, $[Yb_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]$, has a centre of symmetry. The nine-coordinate Yb^{III} atom has a distorted monocapped square antiprismatic geometry. Molecules are linked into three chains by C—H···O hydrogen bonds and π–π stacking interactions [centroid-to-centroid distance 3.775 (4) Å]; combination of the three chains results in the formation of a three-dimensional network.

Related literature

For related literature, see: Liu *et al.* (2007*a*,*b*); Xia *et al.* (2007*a*,*b*,*c*).



Experimental

Crystal data

$[Yb_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]$
M_r = 1817.64
Triclinic, $P\overline{1}$
a = 12.3640 (10) Å
b = 13.5622 (12) Å
c = 13.5954 (13) Å
α = 114.189 (3)°
β = 99.559 (2)°
γ = 103.485 (2)°
V = 1932.3 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.48 mm^{-1}
T = 298 (2) K
0.32 × 0.16 × 0.13 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.505, T_{max} = 0.739
9882 measured reflections
6634 independent reflections
5654 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.089
S = 1.01
6634 reflections
514 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.49 e Å^{-3}
$\Delta\rho_{min}$ = −1.14 e Å^{-3}

Table 1
Selected bond lengths (Å).

Yb1—O1^{i}	2.261 (3)	Yb1—N2	2.494 (4)
Yb1—O3	2.266 (3)	Yb1—O1	2.558 (3)
Yb1—O6	2.300 (4)	Yb1—N1	2.560 (4)
Yb1—O4^{i}	2.311 (3)	Yb1—O5	2.576 (4)
Yb1—O2	2.397 (3)		

Symmetry code: (i) $-x+2, -y+1, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
C30—H30···O6^{ii}	0.93	2.50	3.374 (9)	157
C44—H44···O2^{iii}	0.93	2.44	3.223 (6)	142
C37—H37···O4^{i}	0.93	2.34	2.944 (6)	123
C46—H46···O3	0.93	2.45	3.044 (6)	122

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: AT2427).

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supplementary materials

Acta Cryst. (2007). E**63**, m2795-m2796 [**doi:10.1107/S1600536807051252**]

Tetrakis(μ-naphthalene-1-acetato)bis[(naphthalene-1-acetato)(1,10-phenanthroline)ytterbium(III)]

H.-T. Xia, Y.-F. Liu, D.-Q. Wang and S.-P. Yang

Comment

We have recently reported the crystal structures of the rare earth complexes with 1-naphthylacetic acid (NAA) and 1,10-phenanthroline (phen), $[Eu(NAA)_3(phen)]_2\cdot 2DMF$ (II), $[Gd(NAA)_3(phen)]_2\cdot 2DMF$ (III) (Liu *et al.*, 2007*a*,*b*), $[Pr(NAA)_3(phen)]_2\cdot DMF$, $[Tb(NAA)_3(phen)]_2\cdot 2DMF$ (IV) and $[Sm(NAA)_3(phen)]_2\cdot 2DMF$ (V) (Xia *et al.*, 2007*a*,*b*,*c*). We report here the crystal structure of ytterbium complexes with NAA and phen.

In the title complex, the coordination environment of Yb atom and coordination modes of the NNA ligands coordinated to the Yb^{III} ion are in agreement with the those of we reported (Fig.1). The average bond lengths of between the ytterbium center and carboxylic oxygen atoms are 2.418 (4) Å, shorter than that 2.4725 (5)Å of complex (II), 2.441 (7) of complex (III), 2.450 (7) of complex (IV) and 2.456 (7) of complex (V). The Yb···Yb distance is 3.8482 (5) Å. The dihedral angles of the least-square-plane Yb_2O_2 and naphthyl rings are 66.17 (10)° (C3—C12 ring), 38.48 (12)° (C15—C24 ring) and 69.83 (13)° (C27—C36 ring), and the dihedral angle between Yb_2O_2 plane and phen ring is 73.87 (9)°.

The molecules are linked into two chains running parallel to the *a, b* and *c* axil by means of C—H···O hydrogen bonds and π···π stacking interaction (Fig. 2–4, and Table 2). The ring (C15—C20) in the molecules at (*x*, *y*, *z*) are parallel to one another ring (C15—C20) in the molecules at (2 − *x*, 1 − *y*, 1 − *z*), the separation of ring centroids is 3.775 (4) Å, with an interplanar spacing of *ca* 3.524 Å, corresponding to a ring offset of *ca* 1.358 Å. Combination of the three chains results in the formation of a three-dimensional network.

Experimental

To a stirred solution of 1-naphthylacetic acid (0.5586 g, 3 mmol) and 1,10-phenanthroline monohydrate (0.198 g, 1 mmol) in 30 ml me thanol, and a solution of $Yb(NO_3)_3\cdot 6H_2O$ (0.435 g, 1 mmol) in water (10 ml) was added. The mixed solution was heated to 333 K and stirred for 3 h, and then cooled to room temperature. The precipitate was washed with water and then dissolved in DMF. A colourless crystal suitable for X-ray diffraction was obtained by evaporation of DMF solution.

Refinement

The space group was uniquely assigned from the systematic absences. All H atoms were located in difference Fourier maps. H atoms bonded to C atoms were treated as riding atoms, with C—H distances of 0.93 Å (aryl) and 0.97Å (methylene), and with $U_{iso}(H) = 1.2U_{eq}(C)$ (aryl, methylene).

Figures

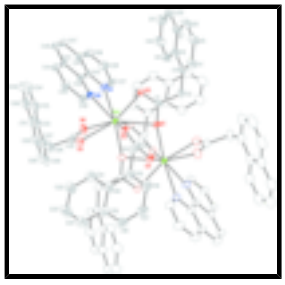


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are at the 30% probability level. Unlabelled atoms in the molecular are related to labelled atoms by (2 − *x*, 1 − *y*, 1 − *z*).

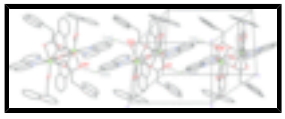


Fig. 2. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···O. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) 2 − *x*, 1 − *y*, 1 − *z*, (B) 1 − *x*, 1 − *y*, 1 − *z*, (C) 1 + *x*, *y*, *z*].

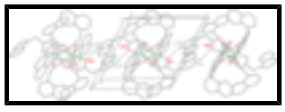


Fig. 3. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···O. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) 2 − *x*, 1 − *y*, 1 − *z*, (D) 2 − *x*, 1 − *y*, 2 − *z*, (E) *x*, *y*, −1 + *z*].

Fig. 4. A larger portion of the crystal structure of (I), showing the formation π···π chain. For clarity, H atoms have been omitted. Dashed lines indicate π···π stacking interactions. [Symmetry codes: (A) 2 − *x*, 1 − *y*, 1 − *z*, (F) *x*, −1 + *y*, *z*, (G) 2 − *x*, 2 − *y*, 1 − *z*].

(I)

Crystal data

$[Yb(C_{12}H_9O_2)_3(C_{12}H_8N_2)]_2$	$Z = 1$
$M_r = 1817.64$	$F_{000} = 910$
Triclinic, $P\overline{1}$	$D_x = 1.562$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 12.3640$ (10) Å	Cell parameters from 5557 reflections
$b = 13.5622$ (12) Å	θ = 2.6–27.6º
$c = 13.5954$ (13) Å	μ = 2.48 mm^{-1}
α = 114.189 (3)º	$T = 298$ (2) K
β = 99.559 (2)º	Block, colourless
γ = 103.485 (2)º	0.32 × 0.16 × 0.13 mm
$V = 1932.3$ (3) Å^3	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	6634 independent reflections
Radiation source: fine-focus sealed tube	5654 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 298(2)$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.7$º

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

T_{min} = 0.505, T_{max} = 0.739

9882 measured reflections

h = −14→14

k = −11→16

l = −16→12

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.031

$wR(F^2)$ = 0.089

S = 1.01

6634 reflections

514 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 2.6017P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 2.49 e Å^{-3}

$\Delta\rho_{min}$ = −1.14 e Å^{-3}

Extinction correction: none

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}
Yb1	0.881165 (17)	0.512900 (17)	0.575054 (18)	0.02437 (8)
N1	0.7210 (4)	0.3782 (4)	0.6034 (4)	0.0326 (10)
N2	0.7069 (3)	0.5728 (3)	0.5967 (4)	0.0313 (10)
O1	0.9257 (3)	0.4061 (3)	0.3906 (3)	0.0307 (8)
O2	0.7461 (3)	0.3720 (3)	0.3952 (3)	0.0348 (8)
O3	0.8872 (3)	0.6166 (3)	0.4798 (3)	0.0306 (8)
O4	1.0443 (3)	0.6260 (3)	0.4177 (3)	0.0328 (8)
O5	0.9358 (3)	0.7207 (3)	0.7312 (3)	0.0434 (9)
O6	0.9222 (4)	0.5761 (3)	0.7664 (3)	0.0468 (10)
C1	0.8185 (4)	0.3510 (4)	0.3426 (4)	0.0293 (11)
C2	0.7816 (5)	0.2586 (5)	0.2208 (5)	0.0395 (13)
H2A	0.8201	0.2907	0.1787	0.047*
H2B	0.8097	0.1969	0.2187	0.047*
C3	0.6525 (5)	0.2077 (5)	0.1606 (5)	0.0414 (13)

C4	0.6084 (5)	0.2365 (5)	0.0817 (5)	0.0501 (15)
H4	0.6583	0.2875	0.0662	0.060*
C5	0.4886 (6)	0.1908 (6)	0.0227 (6)	0.0583 (17)
H5	0.4609	0.2106	−0.0320	0.070*
C6	0.4150 (6)	0.1196 (6)	0.0447 (6)	0.0612 (18)
H6	0.3360	0.0920	0.0066	0.073*
C7	0.4547 (5)	0.0851 (5)	0.1252 (5)	0.0495 (15)
C8	0.5759 (5)	0.1306 (5)	0.1854 (5)	0.0430 (14)
C9	0.6130 (6)	0.0960 (5)	0.2662 (5)	0.0510 (15)
H9	0.6916	0.1236	0.3058	0.061*
C10	0.5366 (6)	0.0233 (6)	0.2872 (6)	0.0618 (18)
H10	0.5630	0.0022	0.3413	0.074*
C11	0.4184 (7)	−0.0201 (6)	0.2284 (7)	0.068 (2)
H11	0.3668	−0.0698	0.2438	0.081*
C12	0.3784 (6)	0.0087 (6)	0.1501 (6)	0.0640 (19)
H12	0.2994	−0.0217	0.1114	0.077*
C13	0.9583 (4)	0.6568 (4)	0.4390 (4)	0.0291 (11)
C14	0.9367 (5)	0.7477 (4)	0.4082 (5)	0.0351 (12)
H14A	0.9074	0.7130	0.3267	0.042*
H14B	0.8759	0.7708	0.4386	0.042*
C15	1.0399 (5)	0.8543 (5)	0.4483 (5)	0.0387 (13)
C16	1.0819 (5)	0.8814 (5)	0.3720 (6)	0.0466 (15)
H16	1.0479	0.8319	0.2953	0.056*
C17	1.1764 (6)	0.9835 (5)	0.4076 (6)	0.0535 (17)
H17	1.2045	0.9992	0.3544	0.064*
C18	1.2249 (6)	1.0567 (5)	0.5175 (6)	0.0549 (17)
H18	1.2864	1.1232	0.5394	0.066*
C19	1.1854 (5)	1.0361 (5)	0.6013 (6)	0.0482 (15)
C20	1.0927 (5)	0.9313 (5)	0.5656 (5)	0.0421 (14)
C21	1.0537 (6)	0.9120 (5)	0.6493 (5)	0.0492 (15)
H21	0.9943	0.8443	0.6283	0.059*
C22	1.1008 (6)	0.9901 (6)	0.7611 (6)	0.0605 (18)
H22	1.0739	0.9748	0.8151	0.073*
C23	1.1890 (7)	1.0925 (6)	0.7941 (7)	0.069 (2)
H23	1.2194	1.1463	0.8701	0.083*
C24	1.2306 (6)	1.1144 (6)	0.7172 (7)	0.0612 (19)
H24	1.2905	1.1826	0.7410	0.073*
C25	0.9414 (5)	0.6813 (5)	0.7993 (5)	0.0418 (13)
C26	0.9737 (7)	0.7631 (5)	0.9259 (5)	0.0581 (18)
H26A	1.0468	0.8232	0.9475	0.070*
H26B	0.9146	0.7991	0.9392	0.070*
C27	0.9852 (6)	0.7079 (6)	0.9998 (5)	0.0554 (17)
C28	1.0934 (7)	0.7158 (6)	1.0531 (6)	0.069 (2)
H28	1.1588	0.7585	1.0450	0.083*
C29	1.1075 (8)	0.6604 (7)	1.1201 (6)	0.073 (2)
H29	1.1816	0.6647	1.1534	0.087*
C30	1.0150 (8)	0.6021 (6)	1.1356 (6)	0.069 (2)
H30	1.0258	0.5667	1.1805	0.083*
C31	0.9002 (7)	0.5926 (6)	1.0854 (6)	0.0613 (19)

C32	0.8846 (6)	0.6445 (5)	1.0150 (5)	0.0537 (16)
C33	0.7711 (7)	0.6308 (6)	0.9613 (6)	0.066 (2)
H33	0.7585	0.6624	0.9131	0.079*
C34	0.6784 (8)	0.5703 (7)	0.9804 (7)	0.082 (3)
H34	0.6029	0.5615	0.9455	0.099*
C35	0.6970 (9)	0.5221 (7)	1.0519 (8)	0.088 (3)
H35	0.6331	0.4814	1.0637	0.106*
C36	0.8016 (9)	0.5324 (7)	1.1029 (7)	0.077 (2)
H36	0.8112	0.5001	1.1508	0.092*
C37	0.7234 (5)	0.2798 (5)	0.5988 (5)	0.0405 (13)
H37	0.7830	0.2536	0.5772	0.049*
C38	0.6399 (5)	0.2131 (5)	0.6249 (5)	0.0481 (15)
H38	0.6435	0.1432	0.6190	0.058*
C39	0.5538 (5)	0.2509 (5)	0.6590 (5)	0.0467 (15)
H39	0.5000	0.2089	0.6798	0.056*
C40	0.5460 (5)	0.3540 (5)	0.6627 (5)	0.0398 (13)
C41	0.6314 (4)	0.4146 (4)	0.6319 (4)	0.0332 (12)
C42	0.6247 (4)	0.5169 (4)	0.6283 (4)	0.0314 (11)
C43	0.5323 (5)	0.5566 (5)	0.6564 (5)	0.0383 (13)
C44	0.5260 (5)	0.6549 (5)	0.6485 (5)	0.0436 (14)
H44	0.4653	0.6822	0.6646	0.052*
C45	0.6089 (5)	0.7103 (5)	0.6174 (5)	0.0434 (14)
H45	0.6065	0.7765	0.6132	0.052*
C46	0.6986 (5)	0.6663 (5)	0.5914 (5)	0.0390 (13)
H46	0.7546	0.7045	0.5695	0.047*
C47	0.4542 (5)	0.3976 (5)	0.6924 (5)	0.0488 (15)
H47	0.3988	0.3589	0.7145	0.059*
C48	0.4477 (5)	0.4935 (5)	0.6885 (5)	0.0481 (15)
H48	0.3870	0.5195	0.7071	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Yb1	0.01897 (12)	0.02730 (12)	0.03045 (13)	0.01066 (8)	0.01018 (8)	0.01416 (9)
N1	0.029 (2)	0.037 (2)	0.042 (3)	0.0146 (19)	0.019 (2)	0.024 (2)
N2	0.025 (2)	0.033 (2)	0.038 (2)	0.0116 (18)	0.0128 (19)	0.016 (2)
O1	0.0185 (17)	0.0326 (18)	0.040 (2)	0.0082 (14)	0.0064 (15)	0.0167 (16)
O2	0.0201 (18)	0.040 (2)	0.035 (2)	0.0084 (15)	0.0116 (15)	0.0088 (17)
O3	0.0274 (18)	0.0360 (19)	0.039 (2)	0.0165 (15)	0.0166 (16)	0.0219 (17)
O4	0.0295 (19)	0.0375 (19)	0.048 (2)	0.0191 (16)	0.0195 (17)	0.0274 (18)
O5	0.040 (2)	0.044 (2)	0.044 (2)	0.0118 (18)	0.0139 (18)	0.0187 (19)
O6	0.065 (3)	0.037 (2)	0.034 (2)	0.0130 (19)	0.016 (2)	0.0136 (18)
C1	0.024 (3)	0.030 (3)	0.034 (3)	0.010 (2)	0.008 (2)	0.016 (2)
C2	0.032 (3)	0.043 (3)	0.037 (3)	0.014 (2)	0.010 (2)	0.012 (3)
C3	0.038 (3)	0.041 (3)	0.040 (3)	0.014 (3)	0.009 (3)	0.014 (3)
C4	0.047 (4)	0.049 (4)	0.044 (4)	0.012 (3)	0.005 (3)	0.018 (3)
C5	0.053 (4)	0.055 (4)	0.052 (4)	0.012 (3)	−0.003 (3)	0.022 (3)
C6	0.048 (4)	0.054 (4)	0.058 (4)	0.010 (3)	−0.003 (3)	0.015 (3)

C7	0.042 (3)	0.043 (3)	0.051 (4)	0.012 (3)	0.009 (3)	0.014 (3)
C8	0.041 (3)	0.039 (3)	0.043 (3)	0.016 (3)	0.011 (3)	0.013 (3)
C9	0.050 (4)	0.044 (3)	0.051 (4)	0.016 (3)	0.008 (3)	0.018 (3)
C10	0.068 (5)	0.050 (4)	0.061 (5)	0.015 (3)	0.011 (4)	0.026 (3)
C11	0.064 (5)	0.054 (4)	0.067 (5)	0.005 (4)	0.016 (4)	0.022 (4)
C12	0.052 (4)	0.052 (4)	0.066 (5)	0.007 (3)	0.012 (4)	0.016 (4)
C13	0.029 (3)	0.029 (3)	0.038 (3)	0.017 (2)	0.012 (2)	0.020 (2)
C14	0.036 (3)	0.038 (3)	0.046 (3)	0.021 (2)	0.017 (3)	0.027 (3)
C15	0.040 (3)	0.036 (3)	0.056 (4)	0.024 (2)	0.019 (3)	0.027 (3)
C16	0.050 (4)	0.042 (3)	0.061 (4)	0.024 (3)	0.025 (3)	0.028 (3)
C17	0.053 (4)	0.046 (4)	0.075 (5)	0.020 (3)	0.030 (4)	0.035 (4)
C18	0.045 (4)	0.044 (4)	0.079 (5)	0.016 (3)	0.020 (4)	0.031 (4)
C19	0.043 (3)	0.038 (3)	0.068 (4)	0.022 (3)	0.010 (3)	0.027 (3)
C20	0.041 (3)	0.040 (3)	0.057 (4)	0.024 (3)	0.016 (3)	0.027 (3)
C21	0.049 (4)	0.042 (3)	0.058 (4)	0.020 (3)	0.012 (3)	0.024 (3)
C22	0.065 (5)	0.052 (4)	0.060 (4)	0.023 (3)	0.011 (4)	0.023 (4)
C23	0.066 (5)	0.052 (4)	0.069 (5)	0.025 (4)	0.000 (4)	0.015 (4)
C24	0.055 (4)	0.044 (4)	0.076 (5)	0.020 (3)	0.005 (4)	0.024 (4)
C25	0.046 (3)	0.046 (3)	0.037 (3)	0.015 (3)	0.021 (3)	0.019 (3)
C26	0.076 (5)	0.047 (4)	0.042 (4)	0.016 (3)	0.023 (3)	0.012 (3)
C27	0.071 (5)	0.052 (4)	0.036 (3)	0.021 (3)	0.018 (3)	0.013 (3)
C28	0.075 (5)	0.065 (5)	0.045 (4)	0.019 (4)	0.017 (4)	0.008 (4)
C29	0.080 (6)	0.071 (5)	0.047 (4)	0.037 (5)	0.006 (4)	0.007 (4)
C30	0.097 (6)	0.060 (5)	0.040 (4)	0.030 (4)	0.010 (4)	0.015 (3)
C31	0.083 (5)	0.051 (4)	0.040 (4)	0.020 (4)	0.022 (4)	0.013 (3)
C32	0.074 (5)	0.049 (4)	0.035 (3)	0.022 (3)	0.020 (3)	0.014 (3)
C33	0.075 (5)	0.060 (4)	0.048 (4)	0.019 (4)	0.019 (4)	0.013 (3)
C34	0.075 (6)	0.075 (5)	0.062 (5)	0.014 (4)	0.019 (4)	0.006 (4)
C35	0.094 (7)	0.071 (5)	0.063 (6)	0.002 (5)	0.027 (5)	0.011 (5)
C36	0.098 (7)	0.063 (5)	0.051 (5)	0.013 (5)	0.023 (5)	0.018 (4)
C37	0.032 (3)	0.045 (3)	0.055 (4)	0.018 (2)	0.017 (3)	0.028 (3)
C38	0.040 (3)	0.048 (3)	0.066 (4)	0.013 (3)	0.016 (3)	0.037 (3)
C39	0.036 (3)	0.052 (4)	0.058 (4)	0.008 (3)	0.019 (3)	0.033 (3)
C40	0.029 (3)	0.049 (3)	0.047 (3)	0.010 (2)	0.017 (3)	0.027 (3)
C41	0.023 (3)	0.043 (3)	0.039 (3)	0.013 (2)	0.014 (2)	0.023 (3)
C42	0.023 (3)	0.042 (3)	0.037 (3)	0.017 (2)	0.013 (2)	0.019 (2)
C43	0.027 (3)	0.046 (3)	0.042 (3)	0.016 (2)	0.015 (2)	0.016 (3)
C44	0.027 (3)	0.045 (3)	0.051 (4)	0.021 (3)	0.013 (3)	0.011 (3)
C45	0.034 (3)	0.038 (3)	0.056 (4)	0.020 (3)	0.015 (3)	0.015 (3)
C46	0.031 (3)	0.040 (3)	0.049 (3)	0.016 (2)	0.014 (3)	0.021 (3)
C47	0.034 (3)	0.056 (4)	0.057 (4)	0.012 (3)	0.022 (3)	0.026 (3)
C48	0.028 (3)	0.054 (4)	0.057 (4)	0.016 (3)	0.022 (3)	0.018 (3)

Geometric parameters (Å, °)

Yb1—O1^{i}	2.261 (3)	C18—C19	1.413 (9)
Yb1—O3	2.266 (3)	C18—H18	0.9300
Yb1—O6	2.300 (4)	C19—C24	1.408 (9)
Yb1—O4^{i}	2.311 (3)	C19—C20	1.435 (8)

Yb1—O2	2.397 (3)	C20—C21	1.401 (8)
Yb1—N2	2.494 (4)	C21—C22	1.368 (9)
Yb1—O1	2.558 (3)	C21—H21	0.9300
Yb1—N1	2.560 (4)	C22—C23	1.393 (10)
Yb1—O5	2.576 (4)	C22—H22	0.9300
Yb1—Yb1^{i}	3.8482 (5)	C23—C24	1.345 (10)
N1—C37	1.316 (6)	C23—H23	0.9300
N1—C41	1.364 (6)	C24—H24	0.9300
N2—C46	1.326 (7)	C25—C26	1.534 (8)
N2—C42	1.358 (6)	C26—C27	1.487 (9)
O1—C1	1.262 (6)	C26—H26A	0.9700
O1—Yb1^{i}	2.261 (3)	C26—H26B	0.9700
O2—C1	1.249 (6)	C27—C28	1.368 (10)
O3—C13	1.251 (6)	C27—C32	1.434 (9)
O4—C13	1.264 (6)	C28—C29	1.413 (11)
O4—Yb1^{i}	2.311 (3)	C28—H28	0.9300
O5—C25	1.245 (7)	C29—C30	1.332 (11)
O6—C25	1.255 (7)	C29—H29	0.9300
C1—C2	1.517 (7)	C30—C31	1.421 (11)
C2—C3	1.511 (8)	C30—H30	0.9300
C2—H2A	0.9700	C31—C36	1.414 (11)
C2—H2B	0.9700	C31—C32	1.415 (9)
C3—C4	1.361 (8)	C32—C33	1.402 (10)
C3—C8	1.427 (8)	C33—C34	1.374 (11)
C4—C5	1.411 (9)	C33—H33	0.9300
C4—H4	0.9300	C34—C35	1.392 (13)
C5—C6	1.329 (9)	C34—H34	0.9300
C5—H5	0.9300	C35—C36	1.308 (12)
C6—C7	1.417 (9)	C35—H35	0.9300
C6—H6	0.9300	C36—H36	0.9300
C7—C12	1.420 (9)	C37—C38	1.402 (8)
C7—C8	1.429 (8)	C37—H37	0.9300
C8—C9	1.412 (8)	C38—C39	1.354 (8)
C9—C10	1.353 (9)	C38—H38	0.9300
C9—H9	0.9300	C39—C40	1.404 (8)
C10—C11	1.395 (10)	C39—H39	0.9300
C10—H10	0.9300	C40—C41	1.410 (7)
C11—C12	1.337 (10)	C40—C47	1.439 (8)
C11—H11	0.9300	C41—C42	1.429 (7)
C12—H12	0.9300	C42—C43	1.416 (7)
C13—C14	1.519 (6)	C43—C44	1.399 (8)
C14—C15	1.509 (7)	C43—C48	1.435 (8)
C14—H14A	0.9700	C44—C45	1.356 (8)
C14—H14B	0.9700	C44—H44	0.9300
C15—C16	1.372 (8)	C45—C46	1.405 (7)
C15—C20	1.426 (8)	C45—H45	0.9300
C16—C17	1.423 (8)	C46—H46	0.9300
C16—H16	0.9300	C47—C48	1.343 (9)

C17—C18	1.337 (9)	C47—H47	0.9300
C17—H17	0.9300	C48—H48	0.9300
O1^{i}—Yb1—O3	77.16 (12)	H14A—C14—H14B	107.3
O1^{i}—Yb1—O6	86.10 (14)	C16—C15—C20	118.6 (5)
O3—Yb1—O6	128.93 (13)	C16—C15—C14	120.4 (5)
O1^{i}—Yb1—O4^{i}	76.78 (12)	C20—C15—C14	120.9 (5)
O3—Yb1—O4^{i}	137.10 (11)	C15—C16—C17	121.5 (6)
O6—Yb1—O4^{i}	82.27 (13)	C15—C16—H16	119.2
O1^{i}—Yb1—O2	125.81 (11)	C17—C16—H16	119.2
O3—Yb1—O2	79.37 (12)	C18—C17—C16	120.0 (6)
O6—Yb1—O2	144.04 (13)	C18—C17—H17	120.0
O4^{i}—Yb1—O2	89.08 (13)	C16—C17—H17	120.0
O1^{i}—Yb1—N2	138.96 (12)	C17—C18—C19	121.9 (6)
O3—Yb1—N2	78.92 (12)	C17—C18—H18	119.0
O6—Yb1—N2	83.60 (15)	C19—C18—H18	119.0
O4^{i}—Yb1—N2	140.13 (13)	C24—C19—C18	123.2 (6)
O2—Yb1—N2	81.01 (12)	C24—C19—C20	118.7 (6)
O1^{i}—Yb1—O1	74.18 (13)	C18—C19—C20	118.1 (6)
O3—Yb1—O1	70.65 (11)	C21—C20—C15	122.5 (5)
O6—Yb1—O1	148.65 (13)	C21—C20—C19	117.6 (6)
O4^{i}—Yb1—O1	69.79 (11)	C15—C20—C19	119.8 (5)
O2—Yb1—O1	52.02 (10)	C22—C21—C20	121.7 (6)
N2—Yb1—O1	127.12 (12)	C22—C21—H21	119.1
O1^{i}—Yb1—N1	147.03 (13)	C20—C21—H21	119.1
O3—Yb1—N1	135.77 (13)	C21—C22—C23	119.9 (7)
O6—Yb1—N1	73.43 (14)	C21—C22—H22	120.0
O4^{i}—Yb1—N1	75.09 (12)	C23—C22—H22	120.0
O2—Yb1—N1	70.61 (13)	C24—C23—C22	120.6 (7)
N2—Yb1—N1	65.16 (13)	C24—C23—H23	119.7
O1—Yb1—N1	111.06 (12)	C22—C23—H23	119.7
O1^{i}—Yb1—O5	74.39 (12)	C23—C24—C19	121.4 (7)
O3—Yb1—O5	76.30 (12)	C23—C24—H24	119.3
O6—Yb1—O5	52.69 (13)	C19—C24—H24	119.3
O4^{i}—Yb1—O5	127.17 (13)	O5—C25—O6	121.2 (5)
O2—Yb1—O5	143.38 (12)	O5—C25—C26	119.3 (5)
N2—Yb1—O5	67.81 (13)	O6—C25—C26	119.5 (5)
O1—Yb1—O5	138.36 (11)	C27—C26—C25	114.7 (5)
N1—Yb1—O5	110.21 (13)	C27—C26—H26A	108.6
O1^{i}—Yb1—Yb1^{i}	39.76 (9)	C25—C26—H26A	108.6
O3—Yb1—Yb1^{i}	69.46 (8)	C27—C26—H26B	108.6
O6—Yb1—Yb1^{i}	121.85 (11)	C25—C26—H26B	108.6
O4^{i}—Yb1—Yb1^{i}	68.65 (8)	H26A—C26—H26B	107.6
O2—Yb1—Yb1^{i}	86.26 (8)	C28—C27—C32	119.2 (7)
N2—Yb1—Yb1^{i}	147.59 (10)	C28—C27—C26	119.6 (7)

O1—Yb1—Yb1^{i}	34.42 (7)	C32—C27—C26	121.2 (7)
N1—Yb1—Yb1^{i}	137.03 (9)	C27—C28—C29	121.2 (8)
O5—Yb1—Yb1^{i}	109.80 (9)	C27—C28—H28	119.4
C37—N1—C41	118.4 (4)	C29—C28—H28	119.4
C37—N1—Yb1	124.1 (3)	C30—C29—C28	120.2 (8)
C41—N1—Yb1	117.4 (3)	C30—C29—H29	119.9
C46—N2—C42	118.4 (4)	C28—C29—H29	119.9
C46—N2—Yb1	121.7 (3)	C29—C30—C31	121.7 (8)
C42—N2—Yb1	119.5 (3)	C29—C30—H30	119.1
C1—O1—Yb1^{i}	163.5 (3)	C31—C30—H30	119.1
C1—O1—Yb1	89.8 (3)	C36—C31—C32	119.3 (8)
Yb1^{i}—O1—Yb1	105.82 (13)	C36—C31—C30	122.1 (8)
C1—O2—Yb1	97.8 (3)	C32—C31—C30	118.6 (7)
C13—O3—Yb1	136.6 (3)	C33—C32—C31	118.6 (7)
C13—O4—Yb1^{i}	136.4 (3)	C33—C32—C27	122.4 (7)
C25—O5—Yb1	86.7 (3)	C31—C32—C27	119.0 (7)
C25—O6—Yb1	99.4 (3)	C34—C33—C32	119.5 (8)
O2—C1—O1	120.3 (5)	C34—C33—H33	120.2
O2—C1—C2	121.7 (4)	C32—C33—H33	120.2
O1—C1—C2	118.0 (4)	C33—C34—C35	120.3 (9)
C3—C2—C1	116.4 (4)	C33—C34—H34	119.8
C3—C2—H2A	108.2	C35—C34—H34	119.8
C1—C2—H2A	108.2	C36—C35—C34	121.9 (9)
C3—C2—H2B	108.2	C36—C35—H35	119.0
C1—C2—H2B	108.2	C34—C35—H35	119.0
H2A—C2—H2B	107.3	C35—C36—C31	120.3 (9)
C4—C3—C8	119.4 (6)	C35—C36—H36	119.9
C4—C3—C2	119.2 (5)	C31—C36—H36	119.9
C8—C3—C2	121.4 (5)	N1—C37—C38	122.7 (5)
C3—C4—C5	121.4 (6)	N1—C37—H37	118.6
C3—C4—H4	119.3	C38—C37—H37	118.6
C5—C4—H4	119.3	C39—C38—C37	119.6 (5)
C6—C5—C4	120.5 (7)	C39—C38—H38	120.2
C6—C5—H5	119.7	C37—C38—H38	120.2
C4—C5—H5	119.7	C38—C39—C40	119.7 (5)
C5—C6—C7	121.2 (6)	C38—C39—H39	120.1
C5—C6—H6	119.4	C40—C39—H39	120.1
C7—C6—H6	119.4	C39—C40—C41	117.3 (5)
C6—C7—C12	122.5 (6)	C39—C40—C47	123.4 (5)
C6—C7—C8	118.8 (6)	C41—C40—C47	119.3 (5)
C12—C7—C8	118.6 (6)	N1—C41—C40	122.2 (5)
C9—C8—C3	123.7 (6)	N1—C41—C42	117.9 (4)
C9—C8—C7	117.7 (6)	C40—C41—C42	119.9 (5)
C3—C8—C7	118.6 (6)	N2—C42—C43	121.8 (5)
C10—C9—C8	121.3 (6)	N2—C42—C41	118.8 (4)
C10—C9—H9	119.3	C43—C42—C41	119.4 (5)
C8—C9—H9	119.3	C44—C43—C42	118.1 (5)
C9—C10—C11	120.5 (7)	C44—C43—C48	122.7 (5)

C9—C10—H10	119.8	C42—C43—C48	119.2 (5)
C11—C10—H10	119.8	C45—C44—C43	119.6 (5)
C12—C11—C10	120.9 (7)	C45—C44—H44	120.2
C12—C11—H11	119.6	C43—C44—H44	120.2
C10—C11—H11	119.6	C44—C45—C46	119.2 (5)
C11—C12—C7	121.0 (7)	C44—C45—H45	120.4
C11—C12—H12	119.5	C46—C45—H45	120.4
C7—C12—H12	119.5	N2—C46—C45	123.0 (5)
O3—C13—O4	125.9 (4)	N2—C46—H46	118.5
O3—C13—C14	117.0 (4)	C45—C46—H46	118.5
O4—C13—C14	117.1 (4)	C48—C47—C40	120.7 (5)
C15—C14—C13	116.5 (4)	C48—C47—H47	119.6
C15—C14—H14A	108.2	C40—C47—H47	119.6
C13—C14—H14A	108.2	C47—C48—C43	121.5 (5)
C15—C14—H14B	108.2	C47—C48—H48	119.3
C13—C14—H14B	108.2	C43—C48—H48	119.3
$O1^{i}$—Yb1—N1—C37	−40.6 (5)	C2—C3—C8—C7	−179.8 (5)
O3—Yb1—N1—C37	136.1 (4)	C6—C7—C8—C9	179.2 (6)
O6—Yb1—N1—C37	−94.5 (4)	C12—C7—C8—C9	0.5 (8)
$O4^{i}$—Yb1—N1—C37	−8.3 (4)	C6—C7—C8—C3	−1.1 (9)
O2—Yb1—N1—C37	86.1 (4)	C12—C7—C8—C3	−179.8 (5)
N2—Yb1—N1—C37	175.0 (5)	C3—C8—C9—C10	179.5 (6)
O1—Yb1—N1—C37	52.7 (5)	C7—C8—C9—C10	−0.9 (9)
O5—Yb1—N1—C37	−132.9 (4)	C8—C9—C10—C11	0.5 (10)
$Yb1^{i}$—Yb1—N1—C37	24.7 (5)	C9—C10—C11—C12	0.2 (11)
$O1^{i}$—Yb1—N1—C41	135.2 (4)	C10—C11—C12—C7	−0.5 (11)
O3—Yb1—N1—C41	−48.0 (4)	C6—C7—C12—C11	−178.5 (7)
O6—Yb1—N1—C41	81.3 (4)	C8—C7—C12—C11	0.2 (10)
$O4^{i}$—Yb1—N1—C41	167.5 (4)	Yb1—O3—C13—O4	17.9 (8)
O2—Yb1—N1—C41	−98.1 (4)	Yb1—O3—C13—C14	−164.5 (3)
N2—Yb1—N1—C41	−9.2 (4)	$Yb1^{i}$—O4—C13—O3	4.3 (9)
O1—Yb1—N1—C41	−131.5 (4)	$Yb1^{i}$—O4—C13—C14	−173.3 (3)
O5—Yb1—N1—C41	42.9 (4)	O3—C13—C14—C15	132.2 (5)
$Yb1^{i}$—Yb1—N1—C41	−159.5 (3)	O4—C13—C14—C15	−49.9 (7)
$O1^{i}$—Yb1—N2—C46	30.1 (5)	C13—C14—C15—C16	116.9 (6)
O3—Yb1—N2—C46	−25.1 (4)	C13—C14—C15—C20	−65.7 (6)
O6—Yb1—N2—C46	106.6 (4)	C20—C15—C16—C17	0.3 (8)
$O4^{i}$—Yb1—N2—C46	176.4 (4)	C14—C15—C16—C17	177.7 (5)
O2—Yb1—N2—C46	−106.0 (4)	C15—C16—C17—C18	−1.4 (9)
O1—Yb1—N2—C46	−80.3 (4)	C16—C17—C18—C19	0.2 (10)
N1—Yb1—N2—C46	−178.7 (4)	C17—C18—C19—C24	−176.6 (6)
O5—Yb1—N2—C46	54.4 (4)	C17—C18—C19—C20	1.9 (9)
$Yb1^{i}$—Yb1—N2—C46	−37.9 (5)	C16—C15—C20—C21	178.5 (5)
$O1^{i}$—Yb1—N2—C42	−141.8 (3)	C14—C15—C20—C21	1.1 (8)
O3—Yb1—N2—C42	163.0 (4)	C16—C15—C20—C19	1.8 (8)
O6—Yb1—N2—C42	−65.2 (4)	C14—C15—C20—C19	−175.6 (5)

$O4^{i}$—Yb1—N2—C42	4.5 (5)	C24—C19—C20—C21	−1.2 (8)
O2—Yb1—N2—C42	82.1 (4)	C18—C19—C20—C21	−179.7 (5)
O1—Yb1—N2—C42	107.8 (4)	C24—C19—C20—C15	175.7 (5)
N1—Yb1—N2—C42	9.4 (3)	C18—C19—C20—C15	−2.8 (8)
O5—Yb1—N2—C42	−117.4 (4)	C15—C20—C21—C22	−176.1 (6)
$Yb1^{i}$—Yb1—N2—C42	150.3 (3)	C19—C20—C21—C22	0.7 (9)
$O1^{i}$—Yb1—O1—C1	−174.9 (3)	C20—C21—C22—C23	0.7 (10)
O3—Yb1—O1—C1	−93.2 (3)	C21—C22—C23—C24	−1.7 (11)
O6—Yb1—O1—C1	132.1 (3)	C22—C23—C24—C19	1.2 (11)
$O4^{i}$—Yb1—O1—C1	103.7 (3)	C18—C19—C24—C23	178.7 (6)
O2—Yb1—O1—C1	−1.7 (3)	C20—C19—C24—C23	0.2 (9)
N2—Yb1—O1—C1	−34.6 (3)	Yb1—O5—C25—O6	0.6 (6)
N1—Yb1—O1—C1	39.5 (3)	Yb1—O5—C25—C26	179.9 (5)
O5—Yb1—O1—C1	−132.6 (3)	Yb1—O6—C25—O5	−0.7 (6)
$Yb1^{i}$—Yb1—O1—C1	−174.9 (3)	Yb1—O6—C25—C26	180.0 (5)
$O1^{i}$—Yb1—O1—$Yb1^{i}$	0.0	O5—C25—C26—C27	−176.3 (6)
O3—Yb1—O1—$Yb1^{i}$	81.65 (14)	O6—C25—C26—C27	3.0 (9)
O6—Yb1—O1—$Yb1^{i}$	−53.0 (3)	C25—C26—C27—C28	99.6 (7)
$O4^{i}$—Yb1—O1—$Yb1^{i}$	−81.43 (14)	C25—C26—C27—C32	−79.4 (8)
O2—Yb1—O1—$Yb1^{i}$	173.1 (2)	C32—C27—C28—C29	1.7 (10)
N2—Yb1—O1—$Yb1^{i}$	140.23 (14)	C26—C27—C28—C29	−177.3 (6)
N1—Yb1—O1—$Yb1^{i}$	−145.61 (14)	C27—C28—C29—C30	−2.2 (11)
O5—Yb1—O1—$Yb1^{i}$	42.3 (2)	C28—C29—C30—C31	0.6 (11)
$O1^{i}$—Yb1—O2—C1	9.9 (3)	C29—C30—C31—C36	−178.9 (7)
O3—Yb1—O2—C1	75.4 (3)	C29—C30—C31—C32	1.5 (10)
O6—Yb1—O2—C1	−138.5 (3)	C36—C31—C32—C33	−2.4 (9)
$O4^{i}$—Yb1—O2—C1	−63.1 (3)	C30—C31—C32—C33	177.2 (6)
N2—Yb1—O2—C1	155.7 (3)	C36—C31—C32—C27	178.4 (6)
O1—Yb1—O2—C1	1.7 (3)	C30—C31—C32—C27	−2.0 (9)
N1—Yb1—O2—C1	−137.6 (3)	C28—C27—C32—C33	−178.7 (6)
O5—Yb1—O2—C1	124.4 (3)	C26—C27—C32—C33	0.2 (9)
$Yb1^{i}$—Yb1—O2—C1	5.6 (3)	C28—C27—C32—C31	0.5 (9)
$O1^{i}$—Yb1—O3—C13	22.5 (5)	C26—C27—C32—C31	179.4 (6)
O6—Yb1—O3—C13	96.6 (5)	C31—C32—C33—C34	1.7 (10)
$O4^{i}$—Yb1—O3—C13	−31.4 (5)	C27—C32—C33—C34	−179.2 (6)
O2—Yb1—O3—C13	−108.3 (5)	C32—C33—C34—C35	−0.5 (11)
N2—Yb1—O3—C13	168.9 (5)	C33—C34—C35—C36	0.1 (13)
O1—Yb1—O3—C13	−55.0 (5)	C34—C35—C36—C31	−0.8 (13)
N1—Yb1—O3—C13	−155.7 (4)	C32—C31—C36—C35	2.0 (11)
O5—Yb1—O3—C13	99.3 (5)	C30—C31—C36—C35	−177.5 (7)
$Yb1^{i}$—Yb1—O3—C13	−18.3 (4)	C41—N1—C37—C38	−1.9 (8)
$O1^{i}$—Yb1—O5—C25	−97.5 (3)	Yb1—N1—C37—C38	173.9 (4)
O3—Yb1—O5—C25	−177.8 (3)	N1—C37—C38—C39	−1.5 (9)
O6—Yb1—O5—C25	−0.4 (3)	C37—C38—C39—C40	2.9 (9)
$O4^{i}$—Yb1—O5—C25	−38.2 (4)	C38—C39—C40—C41	−1.1 (9)

O2—Yb1—O5—C25	132.5 (3)	C38—C39—C40—C47	176.9 (6)
N2—Yb1—O5—C25	98.8 (3)	C37—N1—C41—C40	3.8 (8)
O1—Yb1—O5—C25	−139.7 (3)	Yb1—N1—C41—C40	−172.3 (4)
N1—Yb1—O5—C25	48.1 (4)	C37—N1—C41—C42	−175.3 (5)
Yb1^{i}—Yb1—O5—C25	−115.9 (3)	Yb1—N1—C41—C42	8.7 (6)
O1^{i}—Yb1—O6—C25	73.7 (4)	C39—C40—C41—N1	−2.3 (8)
O3—Yb1—O6—C25	3.6 (4)	C47—C40—C41—N1	179.7 (5)
O4^{i}—Yb1—O6—C25	150.9 (4)	C39—C40—C41—C42	176.7 (5)
O2—Yb1—O6—C25	−131.5 (3)	C47—C40—C41—C42	−1.3 (8)
N2—Yb1—O6—C25	−66.5 (4)	C46—N2—C42—C43	−0.7 (8)
O1—Yb1—O6—C25	124.1 (4)	Yb1—N2—C42—C43	171.4 (4)
N1—Yb1—O6—C25	−132.5 (4)	C46—N2—C42—C41	178.7 (5)
O5—Yb1—O6—C25	0.4 (3)	Yb1—N2—C42—C41	−9.2 (6)
Yb1^{i}—Yb1—O6—C25	92.0 (4)	N1—C41—C42—N2	0.1 (7)
Yb1—O2—C1—O1	−3.2 (5)	C40—C41—C42—N2	−179.0 (5)
Yb1—O2—C1—C2	176.1 (4)	N1—C41—C42—C43	179.5 (5)
Yb1^{i}—O1—C1—O2	−159.3 (8)	C40—C41—C42—C43	0.4 (8)
Yb1—O1—C1—O2	3.0 (5)	N2—C42—C43—C44	1.4 (8)
Yb1^{i}—O1—C1—C2	21.4 (14)	C41—C42—C43—C44	−178.0 (5)
Yb1—O1—C1—C2	−176.3 (4)	N2—C42—C43—C48	179.7 (5)
O2—C1—C2—C3	10.1 (8)	C41—C42—C43—C48	0.3 (8)
O1—C1—C2—C3	−170.6 (5)	C42—C43—C44—C45	−1.6 (8)
C1—C2—C3—C4	106.3 (6)	C48—C43—C44—C45	−179.9 (6)
C1—C2—C3—C8	−73.3 (7)	C43—C44—C45—C46	1.2 (9)
C8—C3—C4—C5	−0.8 (9)	C42—N2—C46—C45	0.3 (8)
C2—C3—C4—C5	179.6 (5)	Yb1—N2—C46—C45	−171.7 (4)
C3—C4—C5—C6	1.4 (10)	C44—C45—C46—N2	−0.6 (9)
C4—C5—C6—C7	−1.8 (11)	C39—C40—C47—C48	−176.3 (6)
C5—C6—C7—C12	−179.6 (6)	C41—C40—C47—C48	1.6 (9)
C5—C6—C7—C8	1.7 (10)	C40—C47—C48—C43	−0.9 (10)
C4—C3—C8—C9	−179.7 (6)	C44—C43—C48—C47	178.2 (6)
C2—C3—C8—C9	−0.1 (9)	C42—C43—C48—C47	−0.1 (9)
C4—C3—C8—C7	0.7 (8)		

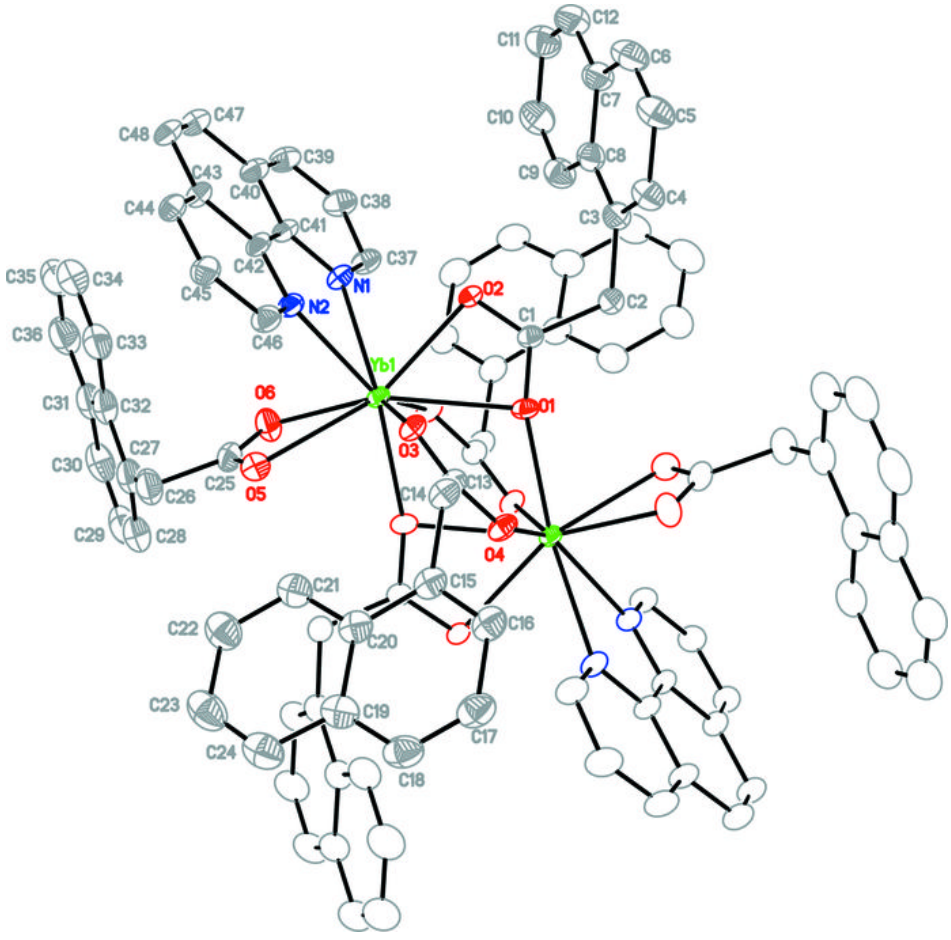
Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C30—H30···O6^{ii}	0.93	2.50	3.374 (9)	157
C44—H44···O2^{iii}	0.93	2.44	3.223 (6)	142
C37—H37···O4^{i}	0.93	2.34	2.944 (6)	123
C46—H46···O3	0.93	2.45	3.044 (6)	122

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

Fig. 1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C40
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Fig. 2

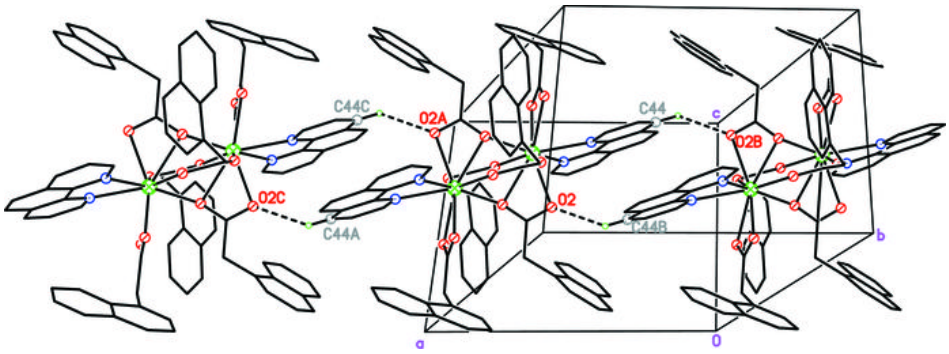

Fig. 3

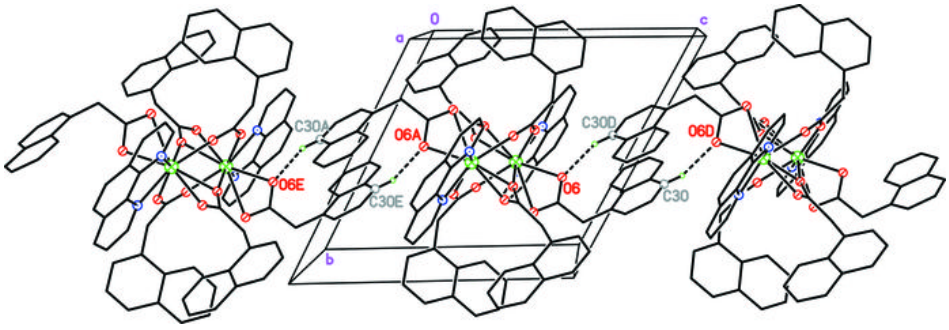
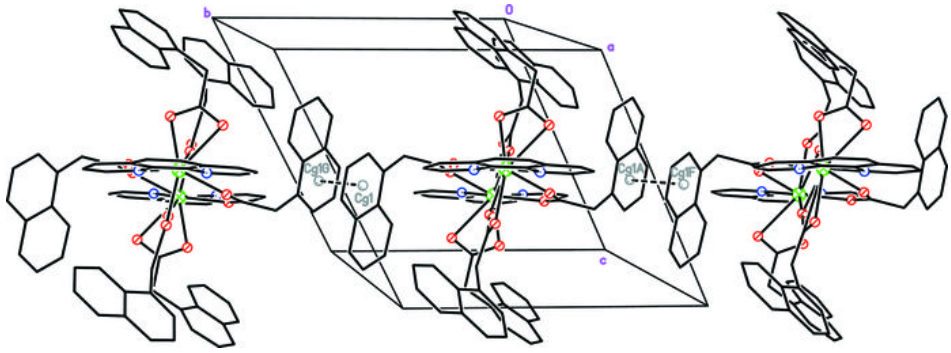
Fig. 4