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# Bis($\mu_2$-2-phenoxypropionato-$\kappa^2O$:$O'$)-bis[(1,10-phenanthroline-$\kappa^2N,N'$)-bis(2-phenoxypropionato-$\kappa^2O,O'$)-ytterbium(III)]

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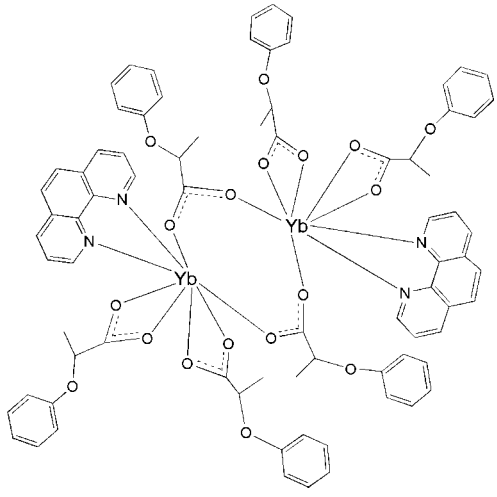
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.030; $wR$ factor = 0.066; data-to-parameter ratio = 13.4.

In the centrosymmetric binuclear title complex, $[Yb_2(C_9H_9O_3)_6(C_{12}H_8N_2)_2]$, the two Yb(III) ions are linked by two 2-phenoxypropionate ($L$) groups in a bidentate bridging mode. Each $Yb^{III}$ ion is eight-coordinated by two O atoms from two bridging $L$ ligands, four O atoms from two chelating $L$ groups and two N atoms from one chelating phen molecule in a distorted $YbN_2O_6$ dodecahedral geometry.

## Related literature

For background to phenoxyalkanoic acids, see: Markus & Buser (1997). For a related Yb complex, see: Lu *et al.* (1999). For compounds with the same formula type but monoclinic symmetry, see: Shen *et al.* (2011*a*) for Tb; Shen *et al.* (2011*b*) for Pr; Shen *et al.* (2011*c*) for Dy; Shen *et al.* (2011*d*) for La; Shen *et al.* (2011*e*) for Ho; Shen *et al.* (2011*f*) for Gd; Shen *et al.* (2011*g*) for Ce.




## Experimental

### Crystal data

$[Yb_2(C_9H_9O_3)_6(C_{12}H_8N_2)_2]$
$M_r$ = 1697.46
Triclinic, $P\overline{1}$
$a$ = 11.3577 (4) Å
$b$ = 12.2091 (5) Å
$c$ = 14.1438 (6) Å
$\alpha$ = 99.111 (2)°
$\beta$ = 91.089 (2)°
$\gamma$ = 114.320 (2)°
$V$ = 1756.94 (12) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 2.72 mm$^{-1}$
$T$ = 296 K
0.32 × 0.20 × 0.06 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.524, $T_{max}$ = 0.849
22731 measured reflections
6187 independent reflections
5246 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.066
$S$ = 1.02
6187 reflections
460 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.00 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.03 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Yb1—O7 | 2.209 (2) | Yb1—O5 | 2.369 (2) |
| Yb1—O8$^{i}$ | 2.266 (3) | Yb1—O2 | 2.403 (3) |
| Yb1—O1 | 2.340 (3) | Yb1—N2 | 2.457 (3) |
| Yb1—O4 | 2.360 (3) | Yb1—N1 | 2.482 (3) |

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

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: *XP* in *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2528).

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Shen, J.-B., Liu, J.-L. & Zhao, G.-L. (2011*g*). *Acta Cryst.* E**67**, m1359–m1360.

# supplementary materials

*Acta Cryst.* (2011). E**67**, m1361 [ **doi:10.1107/S1600536811036105** ]

# Bis($\mu_2$-2-phenoxypropionato-$\kappa^2O$:$O'$)bis[(1,10-phenanthroline-$\kappa^2N$,$N'$)bis(2-phenoxypropionato-$\kappa^2O$,$O'$)ytterbium(III)]

**J.-B. Shen, J.-L. Liu and G.-L. Zhao**

## Comment

The group of phenoxyalkanoic acids includes a considerable number of important herbicides. The desired biological activity is largely dependent on the length of the carbon chain of the alkanoic acid, the nature of the phenoxy group, and the position of its attachment to the carbon chain (Markus & Buser, 1997). The structures of 2-phenoxypropionic acid (H*L*) complexes coupled with their special functionality catched our interest. Here, we describe the $Yb^{III}$ title complex, (I).

The structure of complex (I) is shown in Fig. 1 and the coordination environment of Yb(III) is shown in Fig. 2. The dimeric title compound (I) is centrosymmetric and is comprised of six *L* anions and two phenanthroline ligands. The *L* ligands are coordinated to the $Yb^{III}$ ions in two different modes: chelating and bridging with a Yb—Yb separation of 5.1470 (3) Å. The two Yb(III) ions are linked by two *L* groups through their bidentate bridging modes. Each Yb(III) ion is coordinated to eight atoms, two of which are oxygen atoms from the bridging carboxylates, four oxygen atoms from the bidentate chelating carboxylate groups, and by two nitrogen atoms from a 1,10-phenanthroline molecule. The analysis of structural features indicates that the Yb(III) ion adopts a distorted dodecahedral geometry (Fig. 2), a coordination geometry that is relatively seldom reported for lanthanide carboxylate complexes (Lu *et al.*, 1999). The Yb—O distances are all within the range 2.209 (2)–2.403 (3) Å, and the Yb—N distances rang from 2.457 (3)–2.482 (3) Å, all of which are within the range of those of other eight-coordinated $Yb^{III}$ complexes with carboxylic donor ligands and 1,10-phenanthroline (Lu *et al.*, 1999).

In contrast to the lighter congeners, the Yb(III) complex adopts triclinic symmetry and the metal atom shows coordination number of eight instead of nine. For isoformular compounds with monoclinic symmetry, see: For Tb (Shen *et al.*, 2011*a*), for Pr (Shen *et al.*, 2011*b*), for Dy (Shen *et al.*, 2011*c*), for La (Shen *et al.*, 2011*d*), for Ho (Shen *et al.*, 2011*e*), for Gd (Shen *et al.*, 2011*f*), for Ce (Shen *et al.*, 2011*g*).

## Experimental

Reagents and solvents used were of commercially available quality and without purified before use. 2-Phenoxypropionic acid (1.5 mmol), $Yb(NO_3)_3{\cdot}6H_2O$ (0.5 mmol) and 1,10-phenanthroline (0.5 mmol) were dissolved in 20 ml enthanol, then 10 ml water were added to the above solution. The mixed solution was stirred for 12 h at room temperature. Finally, the deposit was filtered off and the colourless solution was kept in the open air. Colourless crystals were obtained after several days.

## Refinement

The structure was solved by direct methods and successive Fourier difference synthesis. The H atoms bonded to C and N atoms were positioned geometrically and refined using a riding model [aliphatic C—H =0.96 Å ($U_{iso}$(H) = 1.5$U_{eq}$(C)), aromatic C—H = 0.93 Å ($U_{iso}$(H) = 1.2$U_{eq}$(C))].

## Figures

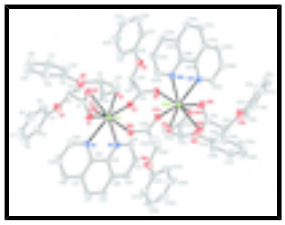

Fig. 1. The molecular structure of the title complex, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

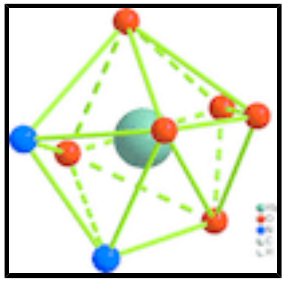

Fig. 2. The coordination environment of the Yb(III).

### Bis(μ$_2$-2-phenoxypropionato-κ$^2$*O*:*O*')bis[(1,10- phenanthroline-κ$^2$*N*,*N*')bis(2-phenoxypropionato-κ$^2$*O*,*O*')ytterbium(III)]

*Crystal data*

| | |
|---|---|
| $[Yb_2(C_9H_9O_3)_6(C_{12}H_8N_2)_2]$ | $Z = 1$ |
| $M_r = 1697.46$ | $F(000) = 850$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.604$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 11.3577$ (4) Å | Cell parameters from 8204 reflections |
| $b = 12.2091$ (5) Å | $\theta = 1.5$–$25.0°$ |
| $c = 14.1438$ (6) Å | $\mu = 2.72$ mm$^{-1}$ |
| $\alpha = 99.111$ (2)° | $T = 296$ K |
| $\beta = 91.089$ (2)° | Block, colourless |
| $\gamma = 114.320$ (2)° | 0.32 × 0.20 × 0.06 mm |
| $V = 1756.94$ (12) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 6187 independent reflections |
| Radiation source: fine-focus sealed tube | 5246 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.039$ |
| phi and ω scans | $\theta_{max} = 25.0°$, $\theta_{min} = 1.5°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -13 \rightarrow 13$ |
| $T_{min} = 0.524$, $T_{max} = 0.849$ | $k = -14 \rightarrow 14$ |
| 22731 measured reflections | $l = -15 \rightarrow 16$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.030$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.066$ | H-atom parameters constrained |
| $S = 1.02$ | $w = 1/[\sigma^2(F_o^2) + (0.0359P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 6187 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 460 parameters | $\Delta\rho_{max} = 1.00$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -1.03$ e Å$^{-3}$ |

*Special details*

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

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Yb1 | 0.321843 (14) | 0.387600 (14) | 0.104334 (12) | 0.03526 (7) |
| O1 | 0.2116 (3) | 0.4766 (3) | 0.2049 (2) | 0.0605 (9) |
| O2 | 0.3679 (3) | 0.4528 (3) | 0.2756 (2) | 0.0598 (8) |
| O3 | 0.1030 (3) | 0.4796 (3) | 0.3790 (2) | 0.0604 (8) |
| O4 | 0.3356 (2) | 0.2126 (2) | 0.1446 (2) | 0.0497 (7) |
| O5 | 0.5181 (2) | 0.3719 (2) | 0.14106 (19) | 0.0427 (6) |
| O7 | 0.4588 (2) | 0.5738 (2) | 0.08986 (19) | 0.0445 (7) |
| O9 | 0.7307 (3) | 0.8066 (2) | 0.2317 (2) | 0.0530 (7) |
| O6 | 0.4646 (3) | 0.1021 (2) | 0.2351 (2) | 0.0520 (7) |
| N1 | 0.0969 (3) | 0.2250 (3) | 0.0782 (2) | 0.0397 (8) |
| N2 | 0.1801 (3) | 0.4252 (3) | −0.0073 (2) | 0.0385 (8) |
| C1 | 0.2746 (4) | 0.4822 (3) | 0.2793 (3) | 0.0424 (10) |
| C17 | 0.3960 (6) | 0.2501 (6) | 0.4604 (4) | 0.0785 (16) |
| H17A | 0.4034 | 0.3258 | 0.4920 | 0.094* |
| C28 | 0.0536 (4) | 0.1309 (4) | 0.1234 (3) | 0.0484 (10) |
| H28A | 0.1087 | 0.1272 | 0.1710 | 0.058* |
| C8 | 0.0119 (6) | 0.1528 (5) | 0.3729 (4) | 0.0816 (16) |
| H8A | 0.0491 | 0.0990 | 0.3795 | 0.098* |

| | | | | |
|---|---|---|---|---|
| C7 | −0.1206 (6) | 0.1093 (5) | 0.3570 (4) | 0.0780 (16) |
| H7A | −0.1729 | 0.0263 | 0.3521 | 0.094* |
| C19 | 0.5677 (3) | 0.6629 (3) | 0.1040 (3) | 0.0334 (8) |
| C16 | 0.3422 (6) | 0.1508 (7) | 0.5030 (4) | 0.102 (2) |
| H16A | 0.3139 | 0.1592 | 0.5639 | 0.123* |
| C4 | 0.0358 (4) | 0.3546 (4) | 0.3711 (3) | 0.0541 (11) |
| C20 | 0.5966 (4) | 0.7492 (3) | 0.2009 (3) | 0.0434 (10) |
| H20A | 0.5496 | 0.7027 | 0.2492 | 0.052* |
| C6 | −0.1743 (6) | 0.1883 (6) | 0.3485 (4) | 0.0882 (17) |
| H6A | −0.2640 | 0.1595 | 0.3382 | 0.106* |
| C9 | 0.0911 (5) | 0.2769 (5) | 0.3792 (4) | 0.0661 (13) |
| H9A | 0.1808 | 0.3059 | 0.3888 | 0.079* |
| C12 | 0.5823 (5) | 0.1475 (4) | 0.1017 (3) | 0.0613 (12) |
| H12A | 0.6322 | 0.1066 | 0.1216 | 0.092* |
| H12B | 0.6354 | 0.2117 | 0.0694 | 0.092* |
| H12C | 0.5089 | 0.0900 | 0.0586 | 0.092* |
| C13 | 0.4271 (4) | 0.1270 (4) | 0.3251 (3) | 0.0519 (11) |
| C18 | 0.4401 (5) | 0.2394 (5) | 0.3698 (3) | 0.0639 (13) |
| H18A | 0.4774 | 0.3072 | 0.3403 | 0.077* |
| C5 | −0.0967 (5) | 0.3113 (5) | 0.3551 (4) | 0.0743 (15) |
| H5A | −0.1341 | 0.3650 | 0.3488 | 0.089* |
| C10 | 0.4573 (4) | 0.2661 (3) | 0.1569 (3) | 0.0394 (9) |
| C32 | −0.1525 (4) | 0.2498 (5) | −0.1287 (4) | 0.0656 (14) |
| H32A | −0.2082 | 0.2559 | −0.1746 | 0.079* |
| C14 | 0.3728 (6) | 0.0264 (5) | 0.3684 (4) | 0.0841 (17) |
| H14A | 0.3656 | −0.0495 | 0.3375 | 0.101* |
| C25 | 0.9109 (6) | 0.6397 (6) | 0.3733 (4) | 0.0799 (17) |
| H25A | 0.9531 | 0.6052 | 0.4077 | 0.096* |
| C24 | 0.7826 (6) | 0.5756 (5) | 0.3430 (4) | 0.0777 (16) |
| H24A | 0.7376 | 0.4977 | 0.3567 | 0.093* |
| C26 | 0.9779 (5) | 0.7534 (6) | 0.3538 (4) | 0.0844 (18) |
| H26A | 1.0659 | 0.7957 | 0.3740 | 0.101* |
| C2 | 0.2398 (4) | 0.5281 (4) | 0.3769 (3) | 0.0493 (11) |
| H2A | 0.2781 | 0.5040 | 0.4280 | 0.059* |
| C15 | 0.3293 (7) | 0.0391 (7) | 0.4574 (5) | 0.117 (3) |
| H15A | 0.2910 | −0.0287 | 0.4867 | 0.141* |
| C39 | 0.0575 (3) | 0.3367 (3) | −0.0342 (3) | 0.0394 (9) |
| C38 | −0.0265 (4) | 0.3479 (4) | −0.1024 (3) | 0.0485 (11) |
| C3 | 0.2877 (5) | 0.6651 (4) | 0.3944 (4) | 0.0704 (14) |
| H3A | 0.2655 | 0.6923 | 0.4561 | 0.106* |
| H3B | 0.2479 | 0.6881 | 0.3452 | 0.106* |
| H3C | 0.3803 | 0.7022 | 0.3931 | 0.106* |
| C34 | 0.1389 (4) | 0.5425 (4) | −0.1136 (3) | 0.0550 (12) |
| H34A | 0.1693 | 0.6142 | −0.1386 | 0.066* |
| C11 | 0.5356 (4) | 0.2010 (3) | 0.1886 (3) | 0.0446 (10) |
| H11A | 0.6109 | 0.2602 | 0.2320 | 0.054* |
| C36 | 0.0142 (3) | 0.2313 (3) | 0.0110 (3) | 0.0394 (9) |
| C30 | −0.1523 (4) | 0.0386 (4) | 0.0319 (3) | 0.0557 (12) |
| H30A | −0.2338 | −0.0258 | 0.0151 | 0.067* |

| | | | | |
|---|---|---|---|---|
| C35 | 0.2173 (4) | 0.5238 (4) | −0.0471 (3) | 0.0469 (10) |
| H35A | 0.3009 | 0.5844 | −0.0295 | 0.056* |
| C22 | 0.7855 (4) | 0.7426 (4) | 0.2753 (3) | 0.0496 (11) |
| C31 | −0.1925 (4) | 0.1492 (5) | −0.0890 (3) | 0.0639 (14) |
| H31A | −0.2737 | 0.0859 | −0.1095 | 0.077* |
| C37 | −0.1128 (4) | 0.1377 (4) | −0.0160 (3) | 0.0516 (11) |
| C33 | 0.0169 (4) | 0.4542 (4) | −0.1415 (3) | 0.0542 (12) |
| H33A | −0.0370 | 0.4647 | −0.1861 | 0.065* |
| C29 | −0.0720 (4) | 0.0362 (4) | 0.1028 (3) | 0.0551 (12) |
| H29A | −0.0996 | −0.0274 | 0.1374 | 0.066* |
| C23 | 0.7186 (5) | 0.6259 (4) | 0.2919 (3) | 0.0609 (13) |
| H23A | 0.6316 | 0.5814 | 0.2692 | 0.073* |
| C27 | 0.9167 (4) | 0.8060 (5) | 0.3046 (4) | 0.0684 (14) |
| H27A | 0.9628 | 0.8838 | 0.2910 | 0.082* |
| C21 | 0.5524 (5) | 0.8474 (4) | 0.1927 (4) | 0.0710 (15) |
| H21A | 0.5703 | 0.9013 | 0.2537 | 0.106* |
| H21B | 0.4608 | 0.8110 | 0.1739 | 0.106* |
| H21C | 0.5978 | 0.8930 | 0.1452 | 0.106* |
| O8 | 0.6489 (3) | 0.6912 (2) | 0.04486 (19) | 0.0453 (7) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Yb1 | 0.02867 (9) | 0.03739 (10) | 0.03569 (11) | 0.00996 (7) | 0.00405 (7) | 0.00639 (7) |
| O1 | 0.0591 (19) | 0.097 (2) | 0.0397 (18) | 0.0519 (19) | −0.0014 (15) | −0.0004 (16) |
| O2 | 0.0611 (19) | 0.089 (2) | 0.0456 (19) | 0.0481 (18) | 0.0087 (15) | 0.0106 (16) |
| O3 | 0.0534 (18) | 0.0599 (19) | 0.071 (2) | 0.0267 (16) | 0.0227 (16) | 0.0109 (16) |
| O4 | 0.0355 (15) | 0.0439 (15) | 0.066 (2) | 0.0119 (13) | −0.0028 (13) | 0.0142 (14) |
| O5 | 0.0335 (13) | 0.0398 (15) | 0.0534 (18) | 0.0121 (12) | 0.0092 (12) | 0.0127 (13) |
| O7 | 0.0409 (15) | 0.0359 (14) | 0.0478 (17) | 0.0080 (13) | −0.0015 (12) | 0.0066 (12) |
| O9 | 0.0450 (16) | 0.0472 (16) | 0.0534 (19) | 0.0086 (14) | −0.0024 (14) | 0.0034 (14) |
| O6 | 0.0615 (18) | 0.0459 (16) | 0.055 (2) | 0.0254 (15) | 0.0140 (15) | 0.0166 (14) |
| N1 | 0.0318 (16) | 0.0412 (18) | 0.042 (2) | 0.0104 (15) | 0.0073 (14) | 0.0094 (16) |
| N2 | 0.0314 (16) | 0.0454 (19) | 0.0349 (19) | 0.0125 (15) | 0.0051 (14) | 0.0068 (15) |
| C1 | 0.038 (2) | 0.040 (2) | 0.048 (3) | 0.0152 (19) | 0.0079 (19) | 0.0087 (19) |
| C17 | 0.090 (4) | 0.099 (4) | 0.057 (4) | 0.054 (4) | 0.005 (3) | 0.003 (3) |
| C28 | 0.042 (2) | 0.047 (2) | 0.055 (3) | 0.015 (2) | 0.014 (2) | 0.015 (2) |
| C8 | 0.103 (5) | 0.073 (4) | 0.074 (4) | 0.043 (4) | 0.016 (3) | 0.011 (3) |
| C7 | 0.083 (4) | 0.064 (3) | 0.074 (4) | 0.017 (3) | 0.029 (3) | 0.015 (3) |
| C19 | 0.034 (2) | 0.0298 (19) | 0.036 (2) | 0.0125 (17) | −0.0005 (18) | 0.0078 (17) |
| C16 | 0.106 (5) | 0.128 (6) | 0.058 (4) | 0.035 (5) | 0.033 (3) | 0.012 (4) |
| C4 | 0.060 (3) | 0.054 (3) | 0.045 (3) | 0.020 (2) | 0.021 (2) | 0.010 (2) |
| C20 | 0.035 (2) | 0.043 (2) | 0.045 (3) | 0.0106 (18) | 0.0050 (18) | 0.0042 (19) |
| C6 | 0.071 (4) | 0.087 (4) | 0.093 (5) | 0.021 (3) | 0.012 (3) | 0.012 (4) |
| C9 | 0.067 (3) | 0.068 (3) | 0.069 (3) | 0.031 (3) | 0.016 (3) | 0.017 (3) |
| C12 | 0.067 (3) | 0.058 (3) | 0.070 (3) | 0.034 (3) | 0.025 (3) | 0.016 (2) |
| C13 | 0.051 (3) | 0.061 (3) | 0.048 (3) | 0.027 (2) | 0.008 (2) | 0.011 (2) |
| C18 | 0.078 (3) | 0.071 (3) | 0.055 (3) | 0.041 (3) | 0.009 (3) | 0.017 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.063 (3) | 0.069 (3) | 0.092 (4) | 0.026 (3) | 0.018 (3) | 0.019 (3) |
| C10 | 0.037 (2) | 0.038 (2) | 0.041 (2) | 0.0151 (19) | 0.0068 (17) | 0.0024 (18) |
| C32 | 0.037 (2) | 0.090 (4) | 0.062 (3) | 0.021 (3) | −0.004 (2) | 0.010 (3) |
| C14 | 0.103 (4) | 0.069 (4) | 0.074 (4) | 0.025 (3) | 0.037 (3) | 0.025 (3) |
| C25 | 0.102 (5) | 0.093 (4) | 0.059 (4) | 0.062 (4) | −0.013 (3) | −0.004 (3) |
| C24 | 0.093 (4) | 0.069 (3) | 0.073 (4) | 0.039 (3) | −0.009 (3) | 0.006 (3) |
| C26 | 0.060 (3) | 0.104 (5) | 0.085 (4) | 0.043 (3) | −0.019 (3) | −0.015 (4) |
| C2 | 0.048 (2) | 0.061 (3) | 0.043 (3) | 0.028 (2) | 0.009 (2) | 0.005 (2) |
| C15 | 0.138 (6) | 0.105 (6) | 0.081 (5) | 0.017 (5) | 0.048 (4) | 0.029 (4) |
| C39 | 0.0292 (19) | 0.050 (2) | 0.037 (2) | 0.0172 (18) | 0.0051 (17) | −0.0026 (19) |
| C38 | 0.031 (2) | 0.071 (3) | 0.042 (3) | 0.022 (2) | 0.0021 (18) | 0.005 (2) |
| C3 | 0.068 (3) | 0.066 (3) | 0.063 (3) | 0.022 (3) | 0.007 (3) | −0.010 (3) |
| C34 | 0.055 (3) | 0.068 (3) | 0.053 (3) | 0.031 (2) | 0.010 (2) | 0.025 (2) |
| C11 | 0.041 (2) | 0.040 (2) | 0.052 (3) | 0.0152 (19) | 0.0049 (19) | 0.011 (2) |
| C36 | 0.0314 (19) | 0.043 (2) | 0.039 (2) | 0.0126 (17) | 0.0082 (17) | 0.0019 (18) |
| C30 | 0.033 (2) | 0.056 (3) | 0.063 (3) | 0.006 (2) | 0.013 (2) | 0.002 (2) |
| C35 | 0.037 (2) | 0.054 (3) | 0.048 (3) | 0.014 (2) | 0.0050 (19) | 0.016 (2) |
| C22 | 0.054 (3) | 0.052 (3) | 0.037 (2) | 0.023 (2) | −0.003 (2) | −0.007 (2) |
| C31 | 0.031 (2) | 0.078 (3) | 0.061 (3) | 0.006 (2) | −0.006 (2) | −0.001 (3) |
| C37 | 0.032 (2) | 0.057 (3) | 0.053 (3) | 0.010 (2) | 0.008 (2) | 0.000 (2) |
| C33 | 0.046 (2) | 0.080 (3) | 0.046 (3) | 0.036 (2) | 0.002 (2) | 0.011 (2) |
| C29 | 0.046 (2) | 0.047 (2) | 0.068 (3) | 0.014 (2) | 0.024 (2) | 0.014 (2) |
| C23 | 0.062 (3) | 0.056 (3) | 0.060 (3) | 0.023 (2) | −0.005 (2) | 0.003 (2) |
| C27 | 0.054 (3) | 0.070 (3) | 0.069 (3) | 0.020 (3) | −0.004 (3) | −0.005 (3) |
| C21 | 0.068 (3) | 0.063 (3) | 0.084 (4) | 0.038 (3) | 0.003 (3) | −0.008 (3) |
| O8 | 0.0413 (15) | 0.0492 (16) | 0.0402 (17) | 0.0146 (13) | 0.0076 (13) | 0.0058 (13) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Yb1—O7 | 2.209 (2) | C12—H12B | 0.9600 |
| Yb1—O8$^{i}$ | 2.266 (3) | C12—H12C | 0.9600 |
| Yb1—O1 | 2.340 (3) | C13—C18 | 1.364 (6) |
| Yb1—O4 | 2.360 (3) | C13—C14 | 1.375 (7) |
| Yb1—O5 | 2.369 (2) | C18—H18A | 0.9300 |
| Yb1—O2 | 2.403 (3) | C5—H5A | 0.9300 |
| Yb1—N2 | 2.457 (3) | C10—C11 | 1.517 (5) |
| Yb1—N1 | 2.482 (3) | C32—C31 | 1.341 (7) |
| Yb1—C10 | 2.703 (4) | C32—C38 | 1.431 (6) |
| Yb1—C1 | 2.720 (4) | C32—H32A | 0.9300 |
| O1—C1 | 1.238 (5) | C14—C15 | 1.371 (8) |
| O2—C1 | 1.249 (4) | C14—H14A | 0.9300 |
| O3—C4 | 1.381 (5) | C25—C26 | 1.357 (8) |
| O3—C2 | 1.420 (5) | C25—C24 | 1.361 (7) |
| O4—C10 | 1.257 (4) | C25—H25A | 0.9300 |
| O5—C10 | 1.248 (4) | C24—C23 | 1.384 (6) |
| O7—C19 | 1.252 (4) | C24—H24A | 0.9300 |
| O9—C22 | 1.384 (5) | C26—C27 | 1.368 (7) |
| O9—C20 | 1.415 (4) | C26—H26A | 0.9300 |
| O6—C13 | 1.378 (5) | C2—C3 | 1.506 (6) |

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|---|---|---|---|
| O6—C11 | 1.418 (5) | C2—H2A | 0.9800 |
| N1—C28 | 1.323 (5) | C15—H15A | 0.9300 |
| N1—C36 | 1.357 (5) | C39—C38 | 1.406 (5) |
| N2—C35 | 1.323 (5) | C39—C36 | 1.434 (5) |
| N2—C39 | 1.365 (4) | C38—C33 | 1.394 (6) |
| C1—C2 | 1.528 (6) | C3—H3A | 0.9600 |
| C17—C16 | 1.357 (8) | C3—H3B | 0.9600 |
| C17—C18 | 1.392 (7) | C3—H3C | 0.9600 |
| C17—H17A | 0.9300 | C34—C33 | 1.361 (6) |
| C28—C29 | 1.405 (6) | C34—C35 | 1.391 (5) |
| C28—H28A | 0.9300 | C34—H34A | 0.9300 |
| C8—C7 | 1.374 (8) | C11—H11A | 0.9800 |
| C8—C9 | 1.394 (7) | C36—C37 | 1.420 (5) |
| C8—H8A | 0.9300 | C30—C29 | 1.355 (6) |
| C7—C6 | 1.355 (7) | C30—C37 | 1.395 (6) |
| C7—H7A | 0.9300 | C30—H30A | 0.9300 |
| C19—O8 | 1.236 (4) | C35—H35A | 0.9300 |
| C19—C20 | 1.528 (5) | C22—C23 | 1.372 (6) |
| C16—C15 | 1.360 (9) | C22—C27 | 1.384 (6) |
| C16—H16A | 0.9300 | C31—C37 | 1.421 (6) |
| C4—C9 | 1.353 (6) | C31—H31A | 0.9300 |
| C4—C5 | 1.374 (6) | C33—H33A | 0.9300 |
| C20—C21 | 1.498 (6) | C29—H29A | 0.9300 |
| C20—H20A | 0.9800 | C23—H23A | 0.9300 |
| C6—C5 | 1.380 (7) | C27—H27A | 0.9300 |
| C6—H6A | 0.9300 | C21—H21A | 0.9600 |
| C9—H9A | 0.9300 | C21—H21B | 0.9600 |
| C12—C11 | 1.509 (6) | C21—H21C | 0.9600 |
| C12—H12A | 0.9600 | O8—Yb1$^{i}$ | 2.266 (3) |
| O7—Yb1—O8$^{i}$ | 91.61 (10) | C11—C12—H12C | 109.5 |
| O7—Yb1—O1 | 87.97 (11) | H12A—C12—H12C | 109.5 |
| O8$^{i}$—Yb1—O1 | 149.93 (10) | H12B—C12—H12C | 109.5 |
| O7—Yb1—O4 | 136.78 (9) | C18—C13—C14 | 121.2 (5) |
| O8$^{i}$—Yb1—O4 | 83.17 (10) | C18—C13—O6 | 124.9 (4) |
| O1—Yb1—O4 | 116.77 (11) | C14—C13—O6 | 114.0 (4) |
| O7—Yb1—O5 | 81.63 (9) | C13—C18—C17 | 118.3 (5) |
| O8$^{i}$—Yb1—O5 | 81.00 (9) | C13—C18—H18A | 120.8 |
| O1—Yb1—O5 | 128.51 (9) | C17—C18—H18A | 120.8 |
| O4—Yb1—O5 | 55.16 (9) | C4—C5—C6 | 120.1 (5) |
| O7—Yb1—O2 | 87.71 (10) | C4—C5—H5A | 120.0 |
| O8$^{i}$—Yb1—O2 | 155.75 (10) | C6—C5—H5A | 120.0 |
| O1—Yb1—O2 | 54.30 (9) | O5—C10—O4 | 121.9 (4) |
| O4—Yb1—O2 | 80.83 (10) | O5—C10—C11 | 117.8 (3) |
| O5—Yb1—O2 | 74.91 (9) | O4—C10—C11 | 120.3 (3) |
| O7—Yb1—N2 | 82.59 (10) | O5—C10—Yb1 | 61.19 (19) |
| O8$^{i}$—Yb1—N2 | 74.23 (10) | O4—C10—Yb1 | 60.76 (19) |
| O1—Yb1—N2 | 75.91 (10) | C11—C10—Yb1 | 178.3 (3) |

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| O4—Yb1—N2 | 135.43 (9) | C31—C32—C38 | 121.7 (4) |
| O5—Yb1—N2 | 150.11 (10) | C31—C32—H32A | 119.1 |
| O2—Yb1—N2 | 129.56 (10) | C38—C32—H32A | 119.1 |
| O7—Yb1—N1 | 148.62 (10) | C15—C14—C13 | 119.4 (6) |
| O8$^{i}$—Yb1—N1 | 87.15 (10) | C15—C14—H14A | 120.3 |
| O1—Yb1—N1 | 77.99 (11) | C13—C14—H14A | 120.3 |
| O4—Yb1—N1 | 74.20 (9) | C26—C25—C24 | 120.6 (5) |
| O5—Yb1—N1 | 128.89 (9) | C26—C25—H25A | 119.7 |
| O2—Yb1—N1 | 105.73 (11) | C24—C25—H25A | 119.7 |
| N2—Yb1—N1 | 66.89 (10) | C25—C24—C23 | 120.3 (5) |
| O7—Yb1—C10 | 109.09 (11) | C25—C24—H24A | 119.9 |
| O8$^{i}$—Yb1—C10 | 81.95 (11) | C23—C24—H24A | 119.9 |
| O1—Yb1—C10 | 126.41 (11) | C25—C26—C27 | 120.4 (5) |
| O4—Yb1—C10 | 27.69 (10) | C25—C26—H26A | 119.8 |
| O5—Yb1—C10 | 27.50 (10) | C27—C26—H26A | 119.8 |
| O2—Yb1—C10 | 75.42 (11) | O3—C2—C3 | 106.3 (4) |
| N2—Yb1—C10 | 153.85 (11) | O3—C2—C1 | 110.4 (3) |
| N1—Yb1—C10 | 101.78 (11) | C3—C2—C1 | 110.7 (4) |
| O7—Yb1—C1 | 88.88 (11) | O3—C2—H2A | 109.8 |
| O8$^{i}$—Yb1—C1 | 176.88 (10) | C3—C2—H2A | 109.8 |
| O1—Yb1—C1 | 27.01 (10) | C1—C2—H2A | 109.8 |
| O4—Yb1—C1 | 98.56 (11) | C16—C15—C14 | 120.1 (7) |
| O5—Yb1—C1 | 102.11 (11) | C16—C15—H15A | 120.0 |
| O2—Yb1—C1 | 27.35 (10) | C14—C15—H15A | 120.0 |
| N2—Yb1—C1 | 102.79 (11) | N2—C39—C38 | 121.8 (4) |
| N1—Yb1—C1 | 90.83 (11) | N2—C39—C36 | 118.1 (3) |
| C10—Yb1—C1 | 100.80 (12) | C38—C39—C36 | 120.1 (3) |
| C1—O1—Yb1 | 93.9 (2) | C33—C38—C39 | 118.4 (4) |
| C1—O2—Yb1 | 90.6 (2) | C33—C38—C32 | 123.0 (4) |
| C4—O3—C2 | 117.9 (3) | C39—C38—C32 | 118.6 (4) |
| C10—O4—Yb1 | 91.5 (2) | C2—C3—H3A | 109.5 |
| C10—O5—Yb1 | 91.3 (2) | C2—C3—H3B | 109.5 |
| C19—O7—Yb1 | 153.0 (2) | H3A—C3—H3B | 109.5 |
| C22—O9—C20 | 118.8 (3) | C2—C3—H3C | 109.5 |
| C13—O6—C11 | 118.7 (3) | H3A—C3—H3C | 109.5 |
| C28—N1—C36 | 117.9 (3) | H3B—C3—H3C | 109.5 |
| C28—N1—Yb1 | 124.4 (3) | C33—C34—C35 | 119.0 (4) |
| C36—N1—Yb1 | 117.7 (2) | C33—C34—H34A | 120.5 |
| C35—N2—C39 | 117.5 (3) | C35—C34—H34A | 120.5 |
| C35—N2—Yb1 | 124.0 (2) | O6—C11—C12 | 106.1 (3) |
| C39—N2—Yb1 | 118.4 (3) | O6—C11—C10 | 114.2 (3) |
| O1—C1—O2 | 121.0 (4) | C12—C11—C10 | 109.3 (3) |
| O1—C1—C2 | 119.5 (4) | O6—C11—H11A | 109.0 |
| O2—C1—C2 | 119.5 (4) | C12—C11—H11A | 109.0 |
| O1—C1—Yb1 | 59.1 (2) | C10—C11—H11A | 109.0 |
| O2—C1—Yb1 | 62.1 (2) | N1—C36—C37 | 122.4 (4) |
| C2—C1—Yb1 | 176.3 (3) | N1—C36—C39 | 118.4 (3) |
| C16—C17—C18 | 120.4 (6) | C37—C36—C39 | 119.2 (4) |

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| C16—C17—H17A | 119.8 | C29—C30—C37 | 120.0 (4) |
| C18—C17—H17A | 119.8 | C29—C30—H30A | 120.0 |
| N1—C28—C29 | 123.1 (4) | C37—C30—H30A | 120.0 |
| N1—C28—H28A | 118.5 | N2—C35—C34 | 123.9 (4) |
| C29—C28—H28A | 118.5 | N2—C35—H35A | 118.0 |
| C7—C8—C9 | 120.6 (6) | C34—C35—H35A | 118.0 |
| C7—C8—H8A | 119.7 | C23—C22—O9 | 124.6 (4) |
| C9—C8—H8A | 119.7 | C23—C22—C27 | 120.3 (4) |
| C6—C7—C8 | 119.5 (5) | O9—C22—C27 | 115.1 (4) |
| C6—C7—H7A | 120.3 | C32—C31—C37 | 121.2 (4) |
| C8—C7—H7A | 120.3 | C32—C31—H31A | 119.4 |
| O8—C19—O7 | 126.0 (3) | C37—C31—H31A | 119.4 |
| O8—C19—C20 | 117.8 (3) | C30—C37—C36 | 117.2 (4) |
| O7—C19—C20 | 116.0 (3) | C30—C37—C31 | 123.6 (4) |
| C17—C16—C15 | 120.6 (6) | C36—C37—C31 | 119.1 (4) |
| C17—C16—H16A | 119.7 | C34—C33—C38 | 119.3 (4) |
| C15—C16—H16A | 119.7 | C34—C33—H33A | 120.3 |
| C9—C4—C5 | 120.3 (5) | C38—C33—H33A | 120.3 |
| C9—C4—O3 | 124.8 (4) | C30—C29—C28 | 119.2 (4) |
| C5—C4—O3 | 114.9 (4) | C30—C29—H29A | 120.4 |
| O9—C20—C21 | 107.7 (3) | C28—C29—H29A | 120.4 |
| O9—C20—C19 | 112.1 (3) | C22—C23—C24 | 119.0 (5) |
| C21—C20—C19 | 109.6 (3) | C22—C23—H23A | 120.5 |
| O9—C20—H20A | 109.1 | C24—C23—H23A | 120.5 |
| C21—C20—H20A | 109.1 | C26—C27—C22 | 119.4 (5) |
| C19—C20—H20A | 109.1 | C26—C27—H27A | 120.3 |
| C7—C6—C5 | 120.3 (5) | C22—C27—H27A | 120.3 |
| C7—C6—H6A | 119.8 | C20—C21—H21A | 109.5 |
| C5—C6—H6A | 119.8 | C20—C21—H21B | 109.5 |
| C4—C9—C8 | 119.2 (5) | H21A—C21—H21B | 109.5 |
| C4—C9—H9A | 120.4 | C20—C21—H21C | 109.5 |
| C8—C9—H9A | 120.4 | H21A—C21—H21C | 109.5 |
| C11—C12—H12A | 109.5 | H21B—C21—H21C | 109.5 |
| C11—C12—H12B | 109.5 | C19—O8—Yb1$^{i}$ | 138.2 (2) |
| H12A—C12—H12B | 109.5 | | |
| O7—Yb1—O1—C1 | −91.5 (2) | C2—O3—C4—C5 | −168.1 (4) |
| O8$^{i}$—Yb1—O1—C1 | 178.8 (2) | C22—O9—C20—C21 | 158.5 (4) |
| O4—Yb1—O1—C1 | 51.5 (3) | C22—O9—C20—C19 | −80.8 (4) |
| O5—Yb1—O1—C1 | −13.9 (3) | O8—C19—C20—O9 | −33.8 (5) |
| O2—Yb1—O1—C1 | −2.9 (2) | O7—C19—C20—O9 | 151.0 (3) |
| N2—Yb1—O1—C1 | −174.4 (3) | O8—C19—C20—C21 | 85.8 (4) |
| N1—Yb1—O1—C1 | 116.7 (3) | O7—C19—C20—C21 | −89.5 (4) |
| C10—Yb1—O1—C1 | 20.9 (3) | C8—C7—C6—C5 | 0.4 (9) |
| O7—Yb1—O2—C1 | 92.0 (2) | C5—C4—C9—C8 | −1.2 (8) |
| O8$^{i}$—Yb1—O2—C1 | −179.2 (2) | O3—C4—C9—C8 | 177.8 (5) |
| O1—Yb1—O2—C1 | 2.8 (2) | C7—C8—C9—C4 | 1.2 (8) |
| O4—Yb1—O2—C1 | −129.8 (2) | C11—O6—C13—C18 | 7.8 (6) |
| O5—Yb1—O2—C1 | 173.9 (3) | C11—O6—C13—C14 | −172.6 (4) |

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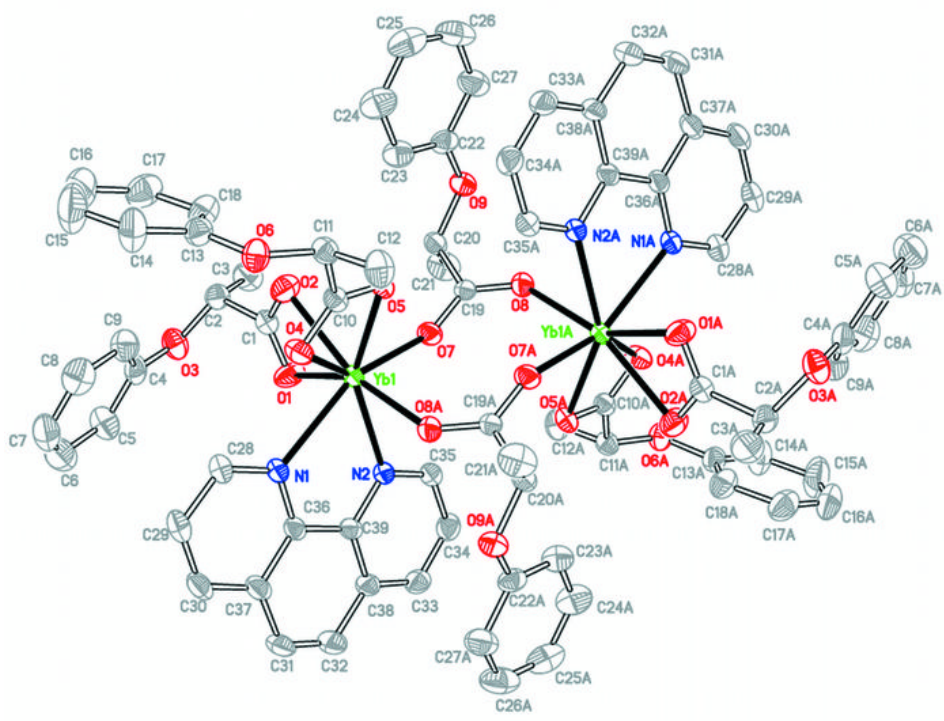
| N2—Yb1—O2—C1 | 13.6 (3) | C14—C13—C18—C17 | −0.4 (7) |
| N1—Yb1—O2—C1 | −59.2 (3) | O6—C13—C18—C17 | 179.1 (4) |
| C10—Yb1—O2—C1 | −157.6 (3) | C16—C17—C18—C13 | 0.3 (8) |
| O7—Yb1—O4—C10 | 0.6 (3) | C9—C4—C5—C6 | 0.9 (8) |
| O8$^{i}$—Yb1—O4—C10 | 85.7 (2) | O3—C4—C5—C6 | −178.3 (5) |
| O1—Yb1—O4—C10 | −118.0 (2) | C7—C6—C5—C4 | −0.5 (9) |
| O5—Yb1—O4—C10 | 1.9 (2) | Yb1—O5—C10—O4 | 3.5 (4) |
| O2—Yb1—O4—C10 | −76.0 (2) | Yb1—O5—C10—C11 | −178.5 (3) |
| N2—Yb1—O4—C10 | 144.9 (2) | Yb1—O4—C10—O5 | −3.5 (4) |
| N1—Yb1—O4—C10 | 174.6 (2) | Yb1—O4—C10—C11 | 178.6 (3) |
| C1—Yb1—O4—C10 | −96.9 (2) | O7—Yb1—C10—O5 | −2.9 (2) |
| O7—Yb1—O5—C10 | 177.2 (2) | O8$^{i}$—Yb1—C10—O5 | 86.0 (2) |
| O8$^{i}$—Yb1—O5—C10 | −89.8 (2) | O1—Yb1—C10—O5 | −105.0 (2) |
| O1—Yb1—O5—C10 | 96.6 (2) | O4—Yb1—C10—O5 | 176.6 (4) |
| O4—Yb1—O5—C10 | −1.9 (2) | O2—Yb1—C10—O5 | −85.3 (2) |
| O2—Yb1—O5—C10 | 87.3 (2) | N2—Yb1—C10—O5 | 110.3 (3) |
| N2—Yb1—O5—C10 | −124.0 (3) | N1—Yb1—C10—O5 | 171.3 (2) |
| N1—Yb1—O5—C10 | −10.9 (3) | C1—Yb1—C10—O5 | −95.5 (2) |
| C1—Yb1—O5—C10 | 90.2 (2) | O7—Yb1—C10—O4 | −179.6 (2) |
| O8$^{i}$—Yb1—O7—C19 | −99.1 (6) | O8$^{i}$—Yb1—C10—O4 | −90.6 (2) |
| O1—Yb1—O7—C19 | 111.0 (6) | O1—Yb1—C10—O4 | 78.4 (3) |
| O4—Yb1—O7—C19 | −17.4 (6) | O5—Yb1—C10—O4 | −176.6 (4) |
| O5—Yb1—O7—C19 | −18.5 (6) | O2—Yb1—C10—O4 | 98.1 (2) |
| O2—Yb1—O7—C19 | 56.6 (6) | N2—Yb1—C10—O4 | −66.3 (4) |
| N2—Yb1—O7—C19 | −173.0 (6) | N1—Yb1—C10—O4 | −5.3 (2) |
| N1—Yb1—O7—C19 | 173.7 (5) | C1—Yb1—C10—O4 | 87.9 (2) |
| C10—Yb1—O7—C19 | −17.1 (6) | C18—C13—C14—C15 | 0.9 (9) |
| C1—Yb1—O7—C19 | 84.0 (6) | O6—C13—C14—C15 | −178.7 (5) |
| O7—Yb1—N1—C28 | −161.8 (3) | C26—C25—C24—C23 | −0.1 (9) |
| O8$^{i}$—Yb1—N1—C28 | 109.8 (3) | C24—C25—C26—C27 | 1.0 (9) |
| O1—Yb1—N1—C28 | −96.5 (3) | C4—O3—C2—C3 | −175.8 (4) |
| O4—Yb1—N1—C28 | 26.1 (3) | C4—O3—C2—C1 | 64.2 (5) |
| O5—Yb1—N1—C28 | 33.8 (4) | O1—C1—C2—O3 | 41.3 (5) |
| O2—Yb1—N1—C28 | −49.3 (3) | O2—C1—C2—O3 | −139.9 (4) |
| N2—Yb1—N1—C28 | −176.1 (3) | O1—C1—C2—C3 | −76.1 (5) |
| C10—Yb1—N1—C28 | 28.7 (3) | O2—C1—C2—C3 | 102.6 (5) |
| C1—Yb1—N1—C28 | −72.5 (3) | C17—C16—C15—C14 | 1.1 (12) |
| O7—Yb1—N1—C36 | 20.3 (4) | C13—C14—C15—C16 | −1.2 (11) |
| O8$^{i}$—Yb1—N1—C36 | −68.1 (3) | C35—N2—C39—C38 | 0.9 (6) |
| O1—Yb1—N1—C36 | 85.6 (3) | Yb1—N2—C39—C38 | −175.8 (3) |
| O4—Yb1—N1—C36 | −151.8 (3) | C35—N2—C39—C36 | −177.7 (3) |
| O5—Yb1—N1—C36 | −144.1 (2) | Yb1—N2—C39—C36 | 5.5 (4) |
| O2—Yb1—N1—C36 | 132.8 (3) | N2—C39—C38—C33 | −1.6 (6) |
| N2—Yb1—N1—C36 | 6.0 (2) | C36—C39—C38—C33 | 177.0 (4) |
| C10—Yb1—N1—C36 | −149.2 (3) | N2—C39—C38—C32 | 178.4 (4) |
| C1—Yb1—N1—C36 | 109.6 (3) | C36—C39—C38—C32 | −3.0 (6) |
| O7—Yb1—N2—C35 | 5.1 (3) | C31—C32—C38—C33 | −179.0 (5) |

| | | | |
|---|---|---|---|
| O8$^{i}$—Yb1—N2—C35 | −88.7 (3) | C31—C32—C38—C39 | 1.0 (7) |
| O1—Yb1—N2—C35 | 94.8 (3) | C13—O6—C11—C12 | 170.1 (3) |
| O4—Yb1—N2—C35 | −151.2 (3) | C13—O6—C11—C10 | −69.4 (4) |
| O5—Yb1—N2—C35 | −53.6 (4) | O5—C10—C11—O6 | 160.0 (3) |
| O2—Yb1—N2—C35 | 85.9 (3) | O4—C10—C11—O6 | −21.9 (5) |
| N1—Yb1—N2—C35 | 177.6 (3) | O5—C10—C11—C12 | −81.3 (4) |
| C10—Yb1—N2—C35 | −113.9 (4) | O4—C10—C11—C12 | 96.7 (4) |
| C1—Yb1—N2—C35 | 92.2 (3) | C28—N1—C36—C37 | −3.9 (6) |
| O7—Yb1—N2—C39 | −178.4 (3) | Yb1—N1—C36—C37 | 174.2 (3) |
| O8$^{i}$—Yb1—N2—C39 | 87.8 (3) | C28—N1—C36—C39 | 176.2 (4) |
| O1—Yb1—N2—C39 | −88.7 (3) | Yb1—N1—C36—C39 | −5.7 (4) |
| O4—Yb1—N2—C39 | 25.3 (3) | N2—C39—C36—N1 | 0.2 (5) |
| O5—Yb1—N2—C39 | 122.9 (3) | C38—C39—C36—N1 | −178.4 (3) |
| O2—Yb1—N2—C39 | −97.6 (3) | N2—C39—C36—C37 | −179.7 (3) |
| N1—Yb1—N2—C39 | −5.9 (2) | C38—C39—C36—C37 | 1.6 (6) |
| C10—Yb1—N2—C39 | 62.6 (4) | C39—N2—C35—C34 | 0.4 (6) |
| C1—Yb1—N2—C39 | −91.3 (3) | Yb1—N2—C35—C34 | 177.0 (3) |
| Yb1—O1—C1—O2 | 5.2 (4) | C33—C34—C35—N2 | −1.0 (7) |
| Yb1—O1—C1—C2 | −176.1 (3) | C20—O9—C22—C23 | −0.5 (6) |
| Yb1—O2—C1—O1 | −5.1 (4) | C20—O9—C22—C27 | −179.1 (4) |
| Yb1—O2—C1—C2 | 176.2 (3) | C38—C32—C31—C37 | 2.4 (8) |
| O7—Yb1—C1—O1 | 87.7 (3) | C29—C30—C37—C36 | 1.8 (6) |
| O4—Yb1—C1—O1 | −135.0 (2) | C29—C30—C37—C31 | −177.9 (4) |
| O5—Yb1—C1—O1 | 168.9 (2) | N1—C36—C37—C30 | 2.0 (6) |
| O2—Yb1—C1—O1 | 174.9 (4) | C39—C36—C37—C30 | −178.1 (4) |
| N2—Yb1—C1—O1 | 5.6 (3) | N1—C36—C37—C31 | −178.2 (4) |
| N1—Yb1—C1—O1 | −60.9 (3) | C39—C36—C37—C31 | 1.7 (6) |
| C10—Yb1—C1—O1 | −163.0 (2) | C32—C31—C37—C30 | 176.0 (5) |
| O7—Yb1—C1—O2 | −87.2 (2) | C32—C31—C37—C36 | −3.8 (7) |
| O1—Yb1—C1—O2 | −174.9 (4) | C35—C34—C33—C38 | 0.3 (7) |
| O4—Yb1—C1—O2 | 50.1 (2) | C39—C38—C33—C34 | 0.9 (6) |
| O5—Yb1—C1—O2 | −6.0 (3) | C32—C38—C33—C34 | −179.1 (4) |
| N2—Yb1—C1—O2 | −169.3 (2) | C37—C30—C29—C28 | −3.6 (7) |
| N1—Yb1—C1—O2 | 124.2 (2) | N1—C28—C29—C30 | 1.7 (7) |
| C10—Yb1—C1—O2 | 22.0 (3) | O9—C22—C23—C24 | −174.9 (4) |
| C36—N1—C28—C29 | 2.0 (6) | C27—C22—C23—C24 | 3.6 (7) |
| Yb1—N1—C28—C29 | −175.9 (3) | C25—C24—C23—C22 | −2.2 (8) |
| C9—C8—C7—C6 | −0.8 (9) | C25—C26—C27—C22 | 0.3 (8) |
| Yb1—O7—C19—O8 | 102.6 (6) | C23—C22—C27—C26 | −2.7 (7) |
| Yb1—O7—C19—C20 | −82.6 (6) | O9—C22—C27—C26 | 176.0 (4) |
| C18—C17—C16—C15 | −0.7 (10) | O7—C19—O8—Yb1$^{i}$ | −7.7 (6) |
| C2—O3—C4—C9 | 12.8 (6) | C20—C19—O8—Yb1$^{i}$ | 177.6 (2) |

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

**Fig. 1**


C25
C26
C27
C24
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C21
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C17
C18
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C14
C13
O6
C11
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C8
O3
C4
O1
Yb1
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C5
C6
O8A
C19A
C28
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N2
C35
C21A
C20A
C36
C39
C29
C34
O9A
C30
C37
C38
C33
C23A
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C10A
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C12A
C11A
O6A
C13A
C15A
C18A
C16A
C17A

**Fig. 2**