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# Poly[hexaaquabis($\mu_3$-terephthalato)($\mu_2$-terephthalato)diytterbium(III)]

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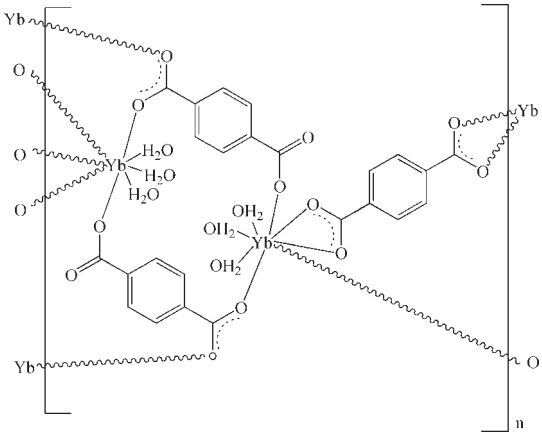
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.020; $wR$ factor = 0.048; data-to-parameter ratio = 11.3.

In the title two-dimensional coordination polymer, $[Yb_2(C_8H_4O_4)_3(H_2O)_6]_n$, the unique $Yb^{III}$ ion is eight-coordinated in a distorted dodecahedral coordination geometry by three water O atoms and five O atoms from carboxylate groups belonging to four different terephthalate ligands. One of the terephthalate ligands is located around an inversion center. The coordination polymers are parallel to (121) and are connected by O—H···O hydrogen bonds into a three-dimensional framework.

## Related literature

For the isostructural erbium(III) and lutetium(III) complexes, see: Daiguebonne *et al.* (2006); Xie *et al.* (2008).




## Experimental

### Crystal data

$[Yb_2(C_8H_4O_4)_3(H_2O)_6]$ $M_r$ = 473.26
Triclinic, $P\overline{1}$
$a$ = 7.8413 (7) Å
$b$ = 9.5545 (8) Å
$c$ = 10.6561 (9) Å
$\alpha$ = 68.827 (1)°
$\beta$ = 71.024 (1)°
$\gamma$ = 75.206 (1)°
$V$ = 695.34 (10) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 6.77 mm$^{-1}$
$T$ = 296 K
0.21 × 0.18 × 0.17 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.251, $T_{max}$ = 0.316
3564 measured reflections
2444 independent reflections
2323 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.015

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.048
$S$ = 1.04
2444 reflections
217 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.82 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.73 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$W$···O2$W^{i}$ | 0.81 (4) | 2.35 (3) | 3.123 (5) | 158 (6) |
| O1$W$—H1$W$···O3 | 0.81 (4) | 2.52 (4) | 3.104 (5) | 130 (4) |
| O1$W$—H2$W$···O5$^{ii}$ | 0.82 (4) | 1.91 (5) | 2.714 (4) | 170 (5) |
| O2$W$—H3$W$···O1$^{iii}$ | 0.82 (5) | 1.97 (5) | 2.771 (4) | 167 (5) |
| O2$W$—H4$W$···O1$^{iv}$ | 0.82 (3) | 2.17 (3) | 2.900 (5) | 149 (5) |
| O3$W$—H5$W$···O6$^{v}$ | 0.82 (3) | 2.08 (2) | 2.846 (4) | 156 (4) |
| O3$W$—H6$W$···O1$^{iv}$ | 0.82 (4) | 1.95 (4) | 2.746 (4) | 165 (5) |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The author acknowledges South China Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2241).

## References

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# supplementary materials

*Acta Cryst.* (2010). E**66**, m33 [ **doi:10.1107/S160053680905171X** ]

# Poly[hexaaquabis($\mu_3$-terephthalato)($\mu_2$-terephthalato)diytterbium(III)]

**S. Feng**

## Comment

Terephthalic acid as a dicarboxylate ligand may exhibit various coordination modes with transition metals or lanthanide ions that result in one-, two- or three-dimensional metal-organic frameworks (MOFs). As an extension of this research we report here the structure of the title two-dimensional coordination polymer of $Yb^{III}$ which is isostructural with $Lu^{III}$ and $Er^{III}$ complexes (Daiguebonne *et al.*, 2006; Xie *et al.*, 2008) .

The asymmetric unit of the title compound (Fig. 1) contains one $Yb^{III}$ ion, one and a half of terephthalate ligand, and three coordinated water molecules. The $Yb^{III}$ ion is eight-coordinate with a dodecahedral coordination polyhedron made of three oxygen atoms from three coordination water molecules and five oxygen atoms from carboxylate groups of four different terephthalate ligands.

The coordination polymers are joined by O—H···O hydrogen bonds between coordinated water molecules and carboxylate groups of terephthalate ligands (Table 1).

## Experimental

A mixture of $AgNO_3$(0.057 g, 0.33 mmol), $Yb_2O_3$(0.116 g, 0.33 mmol), 2-pyrazinecarboxylic acid(0.165 g, 1.33 mmol), terephthalic acid (0.166 g, 1.0 mmol), $H_2O$(7 ml), and $HClO_4$(0.257 mmol)(pH 2) was sealed in a 20 ml Teflon-lined reaction vessel at 443 K for 6 days and then slowly cooled to room temperature. The product was collected by filtration, washed with water and air-dried. Colorless block crystals were suitable for X-ray analysis were obtained.

## Refinement

H atoms bonded to C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C). H atoms of the water molecules were found from difference Fourier maps and refined with restraints imposed on the O-H and H···H distances [O—H = 0.82 (1) Å and H···H = 1.29 (1) Å] and displacement parameters set to 1.5$U_{eq}$(O).

**Figures**

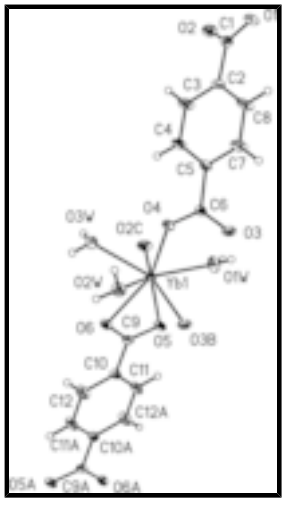


Fig. 1. *ORTEP* view of the asymmetric unit of the title compound with displacement ellipsoids drawn at the 30% probability level. Symmetry codes: (A) 1 - *x*, -*y*, 3 - *z*.;(B) -x, 1 - y, 2 - z; (C) 1 - x, 1 - y, 1 - z.

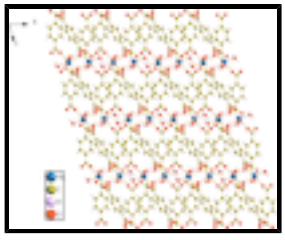

Fig. 2. A view of the three-dimensional structure of the title compound. Hydrogen atoms are omitted for clarity.

**Poly[hexaaquabis(μ$_3$-terephthalato)(μ$_2$-terephthalato)diytterbium(III)]**

*Crystal data*

| | |
|---|---|
| $[Yb_2(C_8H_4O_4)_3(H_2O)_6]$ | $Z = 2$ |
| $M_r = 473.26$ | $F(000) = 452$ |
| Triclinic, $P\overline{1}$ | $D_x = 2.260$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 7.8413$ (7) Å | Cell parameters from 2800 reflections |
| $b = 9.5545$ (8) Å | $\theta = 2.6$–$27.8°$ |
| $c = 10.6561$ (9) Å | $\mu = 6.77$ mm$^{-1}$ |
| $\alpha = 68.8270$ (10)° | $T = 296$ K |
| $\beta = 71.0240$ (10)° | Block, colorless |
| $\gamma = 75.2060$ (10)° | 0.21 × 0.18 × 0.17 mm |
| $V = 695.34$ (10) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII area-detector diffractometer | 2444 independent reflections |
| Radiation source: fine-focus sealed tube | 2323 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.015$ |
| Detector resolution: 0 pixels mm$^{-1}$ | $\theta_{max} = 25.2°$, $\theta_{min} = 2.1°$ |

φ and ω scan

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

$T_{min}$ = 0.251, $T_{max}$ = 0.316

3564 measured reflections

$h = -9 \rightarrow 7$

$k = -10 \rightarrow 11$

$l = -12 \rightarrow 11$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.020$

$wR(F^2) = 0.048$

$S = 1.04$

2444 reflections

217 parameters

9 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 0.8814P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.003$

$\Delta\rho_{max} = 0.82$ e Å$^{-3}$

$\Delta\rho_{min} = -0.73$ 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 | 0.26626 (2) | 0.294523 (19) | 1.006579 (16) | 0.01940 (7) |
| C1 | 0.2794 (6) | 0.7548 (5) | 0.1682 (4) | 0.0244 (9) |
| C2 | 0.2113 (6) | 0.6900 (5) | 0.3233 (4) | 0.0231 (9) |
| C3 | 0.3017 (8) | 0.5574 (6) | 0.3942 (5) | 0.0546 (17) |
| H3 | 0.3999 | 0.5039 | 0.3444 | 0.066* |
| C4 | 0.2506 (8) | 0.5012 (6) | 0.5381 (5) | 0.0501 (15) |
| H4 | 0.3117 | 0.4094 | 0.5839 | 0.060* |
| C5 | 0.1094 (6) | 0.5813 (5) | 0.6133 (4) | 0.0238 (9) |
| C6 | 0.0601 (5) | 0.5283 (5) | 0.7702 (4) | 0.0210 (8) |
| C7 | 0.0173 (7) | 0.7138 (6) | 0.5423 (5) | 0.0465 (14) |
| H7 | −0.0791 | 0.7690 | 0.5917 | 0.056* |
| C8 | 0.0665 (7) | 0.7660 (6) | 0.3982 (5) | 0.0435 (13) |

| | | | | |
|---|---|---|---|---|
| H8 | 0.0001 | 0.8540 | 0.3519 | 0.052* |
| C9 | 0.3969 (5) | 0.1538 (5) | 1.2422 (4) | 0.0221 (9) |
| C10 | 0.4506 (6) | 0.0733 (5) | 1.3751 (4) | 0.0243 (9) |
| C11 | 0.5442 (8) | 0.1424 (5) | 1.4211 (5) | 0.0406 (13) |
| H11 | 0.5754 | 0.2380 | 1.3678 | 0.049* |
| C12 | 0.4091 (8) | −0.0693 (6) | 1.4544 (5) | 0.0411 (13) |
| H12 | 0.3486 | −0.1171 | 1.4234 | 0.049* |
| O1 | 0.1745 (4) | 0.8546 (4) | 0.1024 (3) | 0.0324 (7) |
| O2 | 0.4422 (4) | 0.7076 (4) | 0.1137 (3) | 0.0361 (8) |
| O3 | −0.0475 (4) | 0.6148 (4) | 0.8340 (3) | 0.0317 (7) |
| O4 | 0.1368 (5) | 0.3988 (3) | 0.8290 (3) | 0.0336 (7) |
| O5 | 0.4165 (4) | 0.2898 (3) | 1.1772 (3) | 0.0276 (7) |
| O6 | 0.3249 (4) | 0.0831 (3) | 1.1957 (3) | 0.0271 (7) |
| O1W | 0.3026 (5) | 0.5482 (4) | 0.9349 (4) | 0.0387 (8) |
| H1W | 0.221 (4) | 0.617 (4) | 0.914 (6) | 0.058* |
| H2W | 0.393 (4) | 0.589 (5) | 0.908 (6) | 0.058* |
| O2W | 0.0025 (5) | 0.1676 (4) | 1.0747 (4) | 0.0358 (8) |
| H3W | −0.038 (7) | 0.168 (5) | 1.013 (4) | 0.054* |
| H4W | 0.030 (8) | 0.0778 (19) | 1.115 (5) | 0.054* |
| O3W | 0.3438 (5) | 0.0930 (3) | 0.9110 (3) | 0.0329 (7) |
| H5W | 0.451 (2) | 0.065 (5) | 0.877 (5) | 0.049* |
| H6W | 0.303 (5) | 0.014 (3) | 0.957 (5) | 0.049* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Yb1 | 0.02266 (11) | 0.02072 (11) | 0.01111 (10) | −0.00012 (7) | −0.00580 (7) | −0.00153 (7) |
| C1 | 0.027 (2) | 0.026 (2) | 0.021 (2) | −0.0095 (19) | −0.0056 (18) | −0.0052 (18) |
| C2 | 0.026 (2) | 0.028 (2) | 0.015 (2) | −0.0081 (18) | −0.0059 (16) | −0.0031 (17) |
| C3 | 0.064 (4) | 0.049 (3) | 0.019 (2) | 0.029 (3) | −0.001 (2) | −0.006 (2) |
| C4 | 0.065 (4) | 0.039 (3) | 0.017 (2) | 0.027 (3) | −0.008 (2) | −0.002 (2) |
| C5 | 0.026 (2) | 0.023 (2) | 0.018 (2) | −0.0040 (18) | −0.0057 (17) | −0.0023 (17) |
| C6 | 0.023 (2) | 0.022 (2) | 0.018 (2) | −0.0043 (17) | −0.0086 (17) | −0.0035 (17) |
| C7 | 0.036 (3) | 0.053 (3) | 0.019 (2) | 0.024 (2) | 0.002 (2) | −0.003 (2) |
| C8 | 0.034 (3) | 0.050 (3) | 0.018 (2) | 0.019 (2) | −0.005 (2) | 0.003 (2) |
| C9 | 0.021 (2) | 0.027 (2) | 0.015 (2) | −0.0004 (17) | −0.0046 (16) | −0.0045 (18) |
| C10 | 0.030 (2) | 0.023 (2) | 0.018 (2) | 0.0013 (18) | −0.0117 (17) | −0.0023 (17) |
| C11 | 0.070 (4) | 0.028 (3) | 0.029 (3) | −0.019 (2) | −0.028 (2) | 0.007 (2) |
| C12 | 0.066 (4) | 0.036 (3) | 0.033 (3) | −0.020 (3) | −0.034 (3) | 0.003 (2) |
| O1 | 0.0370 (18) | 0.0362 (18) | 0.0199 (15) | −0.0057 (15) | −0.0127 (14) | 0.0009 (14) |
| O2 | 0.0302 (18) | 0.046 (2) | 0.0226 (16) | −0.0030 (15) | 0.0006 (13) | −0.0083 (15) |
| O3 | 0.0330 (17) | 0.0383 (19) | 0.0170 (15) | 0.0030 (14) | −0.0030 (13) | −0.0094 (14) |
| O4 | 0.054 (2) | 0.0251 (17) | 0.0212 (16) | 0.0009 (15) | −0.0202 (15) | −0.0014 (13) |
| O5 | 0.0352 (17) | 0.0276 (17) | 0.0182 (15) | −0.0074 (13) | −0.0135 (13) | 0.0027 (13) |
| O6 | 0.0391 (18) | 0.0250 (16) | 0.0196 (15) | −0.0059 (13) | −0.0179 (13) | 0.0003 (13) |
| O1W | 0.0313 (18) | 0.0267 (18) | 0.052 (2) | −0.0055 (14) | −0.0105 (17) | −0.0049 (16) |
| O2W | 0.0395 (19) | 0.0379 (19) | 0.0327 (19) | −0.0096 (16) | −0.0140 (15) | −0.0074 (15) |
| O3W | 0.0388 (19) | 0.0277 (17) | 0.0296 (18) | −0.0009 (14) | −0.0077 (15) | −0.0096 (14) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Yb1—O2$^{i}$ | 2.227 (3) | C6—O4 | 1.261 (5) |
| Yb1—O4 | 2.231 (3) | C7—C8 | 1.384 (6) |
| Yb1—O3$^{ii}$ | 2.233 (3) | C7—H7 | 0.9300 |
| Yb1—O1W | 2.327 (3) | C8—H8 | 0.9300 |
| Yb1—O3W | 2.352 (3) | C9—O5 | 1.255 (5) |
| Yb1—O6 | 2.354 (3) | C9—O6 | 1.280 (5) |
| Yb1—O2W | 2.438 (3) | C9—C10 | 1.487 (5) |
| Yb1—O5 | 2.450 (3) | C10—C12 | 1.376 (6) |
| Yb1—C9 | 2.773 (4) | C10—C11 | 1.389 (6) |
| C1—O1 | 1.252 (5) | C11—C12$^{iii}$ | 1.378 (6) |
| C1—O2 | 1.259 (5) | C11—H11 | 0.9300 |
| C1—C2 | 1.502 (5) | C12—C11$^{iii}$ | 1.378 (6) |
| C2—C8 | 1.364 (6) | C12—H12 | 0.9300 |
| C2—C3 | 1.370 (6) | O2—Yb1$^{i}$ | 2.227 (3) |
| C3—C4 | 1.385 (6) | O3—Yb1$^{ii}$ | 2.233 (3) |
| C3—H3 | 0.9300 | O1W—H1W | 0.81 (4) |
| C4—C5 | 1.373 (6) | O1W—H2W | 0.82 (4) |
| C4—H4 | 0.9300 | O2W—H3W | 0.82 (5) |
| C5—C7 | 1.376 (6) | O2W—H4W | 0.82 (3) |
| C5—C6 | 1.507 (5) | O3W—H5W | 0.82 (3) |
| C6—O3 | 1.238 (5) | O3W—H6W | 0.82 (4) |
| O2$^{i}$—Yb1—O4 | 98.80 (12) | C5—C4—C3 | 119.9 (4) |
| O2$^{i}$—Yb1—O3$^{ii}$ | 144.25 (12) | C5—C4—H4 | 120.1 |
| O4—Yb1—O3$^{ii}$ | 98.76 (12) | C3—C4—H4 | 120.1 |
| O2$^{i}$—Yb1—O1W | 76.69 (12) | C4—C5—C7 | 118.6 (4) |
| O4—Yb1—O1W | 77.10 (12) | C4—C5—C6 | 120.8 (4) |
| O3$^{ii}$—Yb1—O1W | 77.26 (12) | C7—C5—C6 | 120.5 (4) |
| O2$^{i}$—Yb1—O3W | 73.41 (12) | O3—C6—O4 | 123.7 (4) |
| O4—Yb1—O3W | 79.48 (11) | O3—C6—C5 | 118.9 (4) |
| O3$^{ii}$—Yb1—O3W | 140.62 (12) | O4—C6—C5 | 117.3 (4) |
| O1W—Yb1—O3W | 138.30 (12) | C5—C7—C8 | 120.8 (4) |
| O2$^{i}$—Yb1—O6 | 94.87 (11) | C5—C7—H7 | 119.6 |
| O4—Yb1—O6 | 148.87 (11) | C8—C7—H7 | 119.6 |
| O3$^{ii}$—Yb1—O6 | 85.72 (11) | C2—C8—C7 | 120.8 (4) |
| O1W—Yb1—O6 | 133.53 (11) | C2—C8—H8 | 119.6 |
| O3W—Yb1—O6 | 77.85 (11) | C7—C8—H8 | 119.6 |
| O2$^{i}$—Yb1—O2W | 143.67 (12) | O5—C9—O6 | 119.7 (4) |
| O4—Yb1—O2W | 74.76 (12) | O5—C9—C10 | 121.4 (4) |
| O3$^{ii}$—Yb1—O2W | 71.38 (12) | O6—C9—C10 | 118.8 (4) |
| O1W—Yb1—O2W | 133.46 (12) | O5—C9—Yb1 | 62.0 (2) |
| O3W—Yb1—O2W | 70.26 (12) | O6—C9—Yb1 | 57.76 (19) |
| O6—Yb1—O2W | 77.66 (11) | C10—C9—Yb1 | 174.7 (3) |

| | | | |
|---|---|---|---|
| O2$^{i}$—Yb1—O5 | 77.29 (11) | C12—C10—C11 | 118.9 (4) |
| O4—Yb1—O5 | 156.47 (11) | C12—C10—C9 | 121.2 (4) |
| O3$^{ii}$—Yb1—O5 | 74.22 (11) | C11—C10—C9 | 119.9 (4) |
| O1W—Yb1—O5 | 79.44 (11) | C12$^{iii}$—C11—C10 | 120.0 (4) |
| O3W—Yb1—O5 | 120.37 (11) | C12$^{iii}$—C11—H11 | 120.0 |
| O6—Yb1—O5 | 54.27 (9) | C10—C11—H11 | 120.0 |
| O2W—Yb1—O5 | 121.90 (10) | C10—C12—C11$^{iii}$ | 121.1 (4) |
| O2$^{i}$—Yb1—C9 | 86.23 (11) | C10—C12—H12 | 119.5 |
| O4—Yb1—C9 | 174.57 (12) | C11$^{iii}$—C12—H12 | 119.5 |
| O3$^{ii}$—Yb1—C9 | 78.02 (11) | C1—O2—Yb1$^{i}$ | 161.1 (3) |
| O1W—Yb1—C9 | 106.19 (13) | C6—O3—Yb1$^{ii}$ | 162.9 (3) |
| O3W—Yb1—C9 | 100.18 (12) | C6—O4—Yb1 | 137.1 (3) |
| O6—Yb1—C9 | 27.39 (11) | C9—O5—Yb1 | 91.1 (2) |
| O2W—Yb1—C9 | 99.99 (11) | C9—O6—Yb1 | 94.8 (2) |
| O5—Yb1—C9 | 26.89 (11) | Yb1—O1W—H1W | 121 (3) |
| O1—C1—O2 | 124.3 (4) | Yb1—O1W—H2W | 132 (3) |
| O1—C1—C2 | 118.7 (4) | H1W—O1W—H2W | 105 (5) |
| O2—C1—C2 | 116.9 (4) | Yb1—O2W—H3W | 118 (4) |
| C8—C2—C3 | 118.3 (4) | Yb1—O2W—H4W | 109 (4) |
| C8—C2—C1 | 121.2 (4) | H3W—O2W—H4W | 105 (5) |
| C3—C2—C1 | 120.3 (4) | Yb1—O3W—H5W | 119 (4) |
| C2—C3—C4 | 121.6 (5) | Yb1—O3W—H6W | 119 (4) |
| C2—C3—H3 | 119.2 | H5W—O3W—H6W | 104 (4) |
| C4—C3—H3 | 119.2 | | |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1W—H1W···O2W$^{ii}$ | 0.81 (4) | 2.35 (3) | 3.123 (5) | 158 (6) |
| O1W—H1W···O3 | 0.81 (4) | 2.52 (4) | 3.104 (5) | 130 (4) |
| O1W—H2W···O5$^{iv}$ | 0.82 (4) | 1.91 (5) | 2.714 (4) | 170 (5) |
| O2W—H3W···O1$^{v}$ | 0.82 (5) | 1.97 (5) | 2.771 (4) | 167 (5) |
| O2W—H4W···O1$^{vi}$ | 0.82 (3) | 2.17 (3) | 2.900 (5) | 149 (5) |
| O3W—H5W···O6$^{vii}$ | 0.82 (3) | 2.08 (2) | 2.846 (4) | 156 (4) |
| O3W—H6W···O1$^{vi}$ | 0.82 (4) | 1.95 (4) | 2.746 (4) | 165 (5) |

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

**Fig. 1**

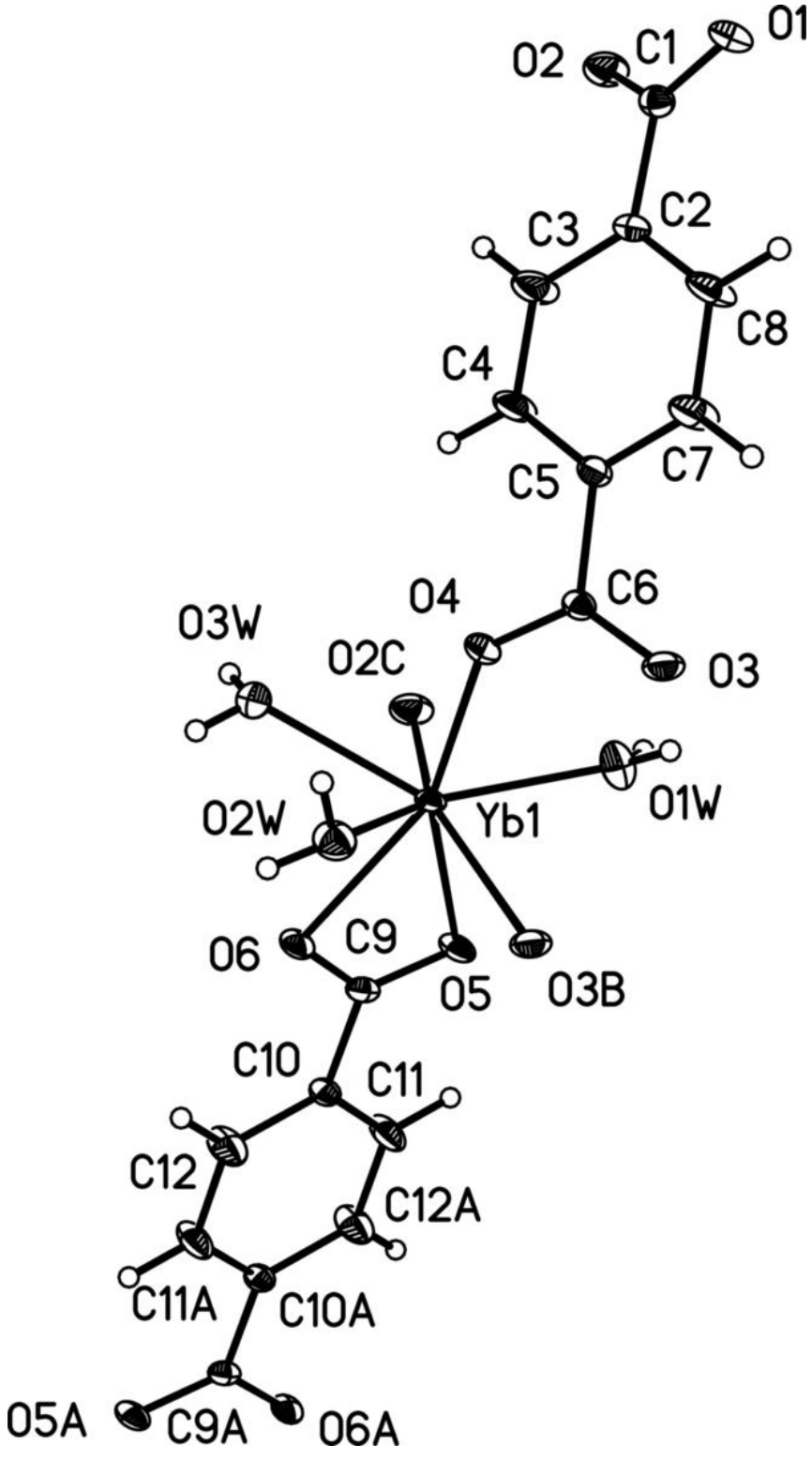
O1
O2
C1
C2
C3
C8
C4
C7
C5
C6
O4
O3W
O2C
O3
O1W
O2W
Yb1
O6
C9
O5
O3B
C10
C11
C12
C12A
C11A
C10A
O5A
C9A
O6A

**Fig. 2**