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# Tris(*N*-acetylglycinato-$\kappa^2O,O'$)triaquaterbium(III)

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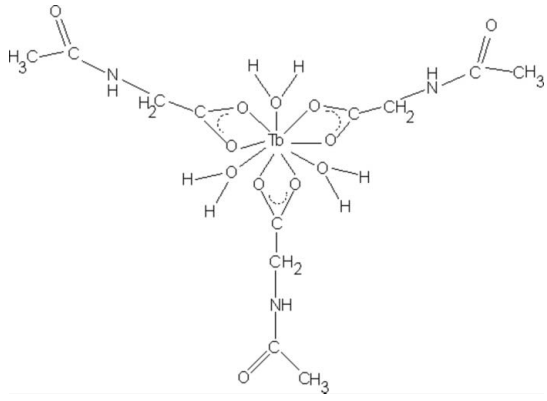
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.015; $wR$ factor = 0.037; data-to-parameter ratio = 8.0.

The title complex, $[Tb(C_4H_6NO_3)_3(H_2O)_3]$, was prepared by reacting terbium carbonate with *N*-acetylglycine in aqueous medium. The $Tb^{III}$ atom is coordinated by nine O atoms, six of them belonging to the three carboxylate groups of the ligands and three to the water molecules. The molecule lies on a threefold rotation axis.

## Related literature

For related compounds, see: Kamath & Udupa (1983); Kameshwar *et al.* (2007); Udupa & Krebs (1978); Zeng & Pan (1992).



## Experimental

### *Crystal data*

$[Tb(C_4H_6NO_3)_3(H_2O)_3]$
$M_r$ = 561.26
Trigonal, $R\overline{3}$
$a$ = 16.540 (4) Å
$c$ = 5.9554 (12) Å
$V$ = 1411.0 (6) Å$^3$
$Z$ = 3
Mo $K\alpha$ radiation
$\mu$ = 3.83 mm$^{-1}$
$T$ = 298 (2) K
0.40 × 0.18 × 0.18 mm

### *Data collection*

Rigaku AFC-7S diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.310, $T_{max}$ = 0.515
1384 measured reflections
892 independent reflections
694 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019
3 standard reflections
every 150 reflections
intensity decay: 1.8%

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.037
$S$ = 1.01
892 reflections
111 parameters
7 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.76 e Å$^{-3}$
Absolute structure: Flack (1983); 172 Friedel pairs
Flack parameter: −0.013 (11)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Tb1—O4 | 2.359 (3) | Tb1—O1 | 2.513 (2) |
| Tb1—O2 | 2.473 (2) | | |
| O4$^i$—Tb1—O4 | 78.52 (11) | O4$^i$—Tb1—O1 | 93.22 (9) |
| O4—Tb1—O2$^i$ | 67.66 (8) | O4—Tb1—O1 | 158.57 (8) |
| O4$^i$—Tb1—O2 | 80.36 (9) | O2—Tb1—O1 | 51.97 (7) |
| O4—Tb1—O2 | 142.98 (9) | O4—Tb1—O1$^i$ | 119.55 (8) |

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

Data collection: *WinAFC* (Rigaku/MSC, 2004); cell refinement: *WinAFC*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2077).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2584 [ **doi:10.1107/S1600536807045618** ]

# Tris(*N*-acetylglycinato-$\kappa^2 O,O'$)triaquaterbium(III)

**P. M. Kameshwar, A. Wadawale and V. R. Ajgaonkar**

## Comment

Rare earth complexes of *N*-acetylglycine were synthesized and reported to be isostructural and hexagonal (Kamath & Udupa, 1983). However, the detailed structural analysis was not given. The crystal structures of neodymium, europium and erbium complexes of *N*-acetylglycine have been reported (Zeng & Pan, 1992). The compounds were found to be isostructural and trigonal.

The structure of the title compound contains a $Tb^{III}$ atom coordinated by six O atoms from three carboxylate groups and three O atoms from water molecules (Fig. 1). The three chelated carboxylate rings are completely staggered. The three Tb—O(water) bonds are also completely staggered with the same angle of 78.5 (1)° between two such bonds (Table 1). The angles O1—C1—O2 are 119.9 (3)°, while the angles subtended at Tb atom by the carboxylate O atoms (O2—Tb1—O1) is 51.97 (7)°. The bond distances between the two carboxylate O atoms and the Tb atom differ by only 0.04 Å. The bond lengths of the two carboxylate O atoms to the C atom differ by only 0.008 Å. The carboxylate group is thus resonance stabilized and functions symmetrically as a bidentate chelate. Apart from the carboxylate group, the bond distances and bond angles of *N*-acetylglycinate moiety in the title compound are not significantly different from those of free *N*-acetylglycine and its copper (Udupa and Krebs, 1978), neodymium, europium and erbium complexes (Zeng & Pan, 1992).

The title compound is isostructural with its samarium (Kameshwar *et al.*, 2007), neodymium, europium and erbium analogues (Zeng & Pan, 1992). The coordination geometry of the title compound can be described in terms of a 4,4,4-tricapped triangular prism. The lattice parameters of the samarium and terbium complexes are in line with the well known lanthanide contraction. Interestingly, the terbium complex is found to be triboluminescent and emit green light on striking the crystals with a spatula or a glass rod when observed in dark.

## Experimental

The title compound was synthesized by adding terbium carbonate (0.397 g, 2.5 mmol) to *N*-acetylglycine (0.878 g, 7.5 mmol) dissolved in 50 ml water and allowing to react on a steam bath till the carbonate dissolved. A few mg of the carbonate was added to ensure that no unreacted acid was present. The unreacted carbonate was filtered off and the filtrate was evaporated naturally at ambient temperature. The crystals suitable for X-ray diffraction were picked up and dried in air. Analysis, calculated for $C_{12}H_{24}N_3O_{12}Tb$: C 25.68, H 4.31, N 7.49, Tb 28.32%; found: C 25.26, H 4.33, N 7.11, Tb 28.05%.

## Refinement

All H atoms were found in difference Fourier maps and refined isotropically.

**Figures**

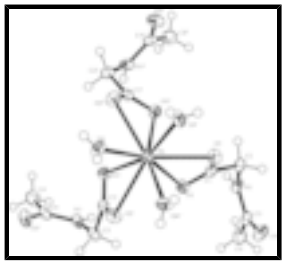


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) −*x* + *y*, −*x*, *z*; (ii) −*y*, *x*-*y*, *z*.]

## Tris(*N*-acetylglycinato-κ$^2$*O*,*O*')triaquaterbium(III)

*Crystal data*

| | |
|---|---|
| $[Tb(C_4H_6NO_3)_3(H_2O)_3]$ | $Z = 3$ |
| $M_r = 561.26$ | $F_{000} = 834$ |
| | $D_x = 1.982$ Mg m$^{-3}$ |
| Trigonal, *R*3 | $D_m = 1.983$ Mg m$^{-3}$ |
| | $D_m$ measured by floatation method |
| Hall symbol: R 3 | Mo *K*α radiation<br>λ = 0.71073 Å |
| *a* = 16.540 (4) Å | Cell parameters from 25 reflections |
| *b* = 16.540 (4) Å | θ = 12.7–16.8º |
| *c* = 5.9554 (12) Å | μ = 3.83 mm$^{-1}$ |
| α = 90º | *T* = 298 (2) K |
| β = 90º | Needle, colourless |
| γ = 120º | 0.40 × 0.18 × 0.18 mm |
| *V* = 1411.0 (6) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Rigaku AFC-7S diffractometer | $R_{int} = 0.019$ |
| Radiation source: fine-focus sealed tube | $\theta_{max} = 27.4$º |
| Monochromator: graphite | $\theta_{min} = 3.7$º |
| *T* = 298(2) K | *h* = −21→18 |
| ω–2θ scans | *k* = 0→21 |
| Absorption correction: ψ scan (North *et al.*, 1968) | *l* = −4→7 |
| $T_{min} = 0.310$, $T_{max} = 0.515$ | 3 standard reflections |
| 1384 measured reflections | every 150 reflections |
| 892 independent reflections | intensity decay: 1.8% |
| 694 reflections with $I > 2\sigma(I)$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: difference Fourier map |

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.015$

$wR(F^2) = 0.037$

$S = 1.01$

892 reflections

111 parameters

7 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.37$ e Å$^{-3}$

$\Delta\rho_{min} = -0.76$ e Å$^{-3}$

Extinction correction: none

Absolute structure: Flack (1983); 172 Friedel pairs

Flack parameter: −0.013 (11)

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C2 | 0.2261 (2) | 0.2052 (2) | 0.2356 (5) | 0.0230 (6) |
| N2 | 0.25512 (18) | 0.1769 (2) | 0.0361 (5) | 0.0238 (5) |
| C3 | 0.3229 (2) | 0.1546 (2) | 0.0448 (5) | 0.0242 (6) |
| O3 | 0.36586 (17) | 0.1634 (2) | 0.2220 (4) | 0.0336 (6) |
| C4 | 0.3410 (3) | 0.1165 (3) | −0.1642 (7) | 0.0343 (8) |
| O4 | −0.1128 (2) | −0.0928 (2) | 0.9043 (4) | 0.0257 (5) |
| H1 | 0.223 (3) | 0.169 (3) | −0.099 (9) | 0.039 (12)* |
| H2B | 0.280 (3) | 0.247 (3) | 0.335 (7) | 0.028 (10)* |
| H2A | 0.190 (3) | 0.234 (3) | 0.202 (8) | 0.041 (12)* |
| H4A | 0.314 (4) | 0.129 (4) | −0.301 (9) | 0.058 (15)* |
| H4C | 0.404 (5) | 0.140 (4) | −0.185 (11) | 0.08 (2)* |
| H4B | 0.314 (4) | 0.051 (4) | −0.169 (10) | 0.065 (18)* |
| H2W | −0.0975 | −0.1118 | 1.0376 | 0.048 (13)* |
| H1W | −0.1653 | −0.1002 | 0.8540 | 0.09 (3)* |
| Tb1 | 0.0000 | 0.0000 | 0.6338 | 0.01496 (6) |
| O1 | 0.11955 (16) | 0.04238 (17) | 0.3289 (4) | 0.0231 (4) |
| O2 | 0.14810 (16) | 0.14866 (16) | 0.5830 (4) | 0.0258 (5) |
| C1 | 0.1632 (3) | 0.1268 (2) | 0.3916 (5) | 0.0173 (5) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C2 | 0.0198 (13) | 0.0239 (14) | 0.0214 (15) | 0.0080 (12) | 0.0025 (12) | 0.0027 (12) |
| N2 | 0.0176 (11) | 0.0309 (14) | 0.0180 (12) | 0.0084 (11) | 0.0003 (10) | 0.0017 (11) |
| C3 | 0.0170 (13) | 0.0237 (15) | 0.0241 (15) | 0.0043 (12) | 0.0038 (12) | 0.0040 (12) |
| O3 | 0.0252 (12) | 0.0481 (15) | 0.0273 (13) | 0.0183 (11) | −0.0041 (10) | 0.0008 (12) |
| C4 | 0.0286 (17) | 0.038 (2) | 0.032 (2) | 0.0134 (15) | 0.0061 (15) | −0.0041 (16) |
| O4 | 0.0211 (13) | 0.0325 (14) | 0.0227 (12) | 0.0126 (12) | 0.0009 (11) | 0.0103 (11) |
| Tb1 | 0.01651 (7) | 0.01651 (7) | 0.01186 (9) | 0.00826 (3) | 0.000 | 0.000 |
| O1 | 0.0244 (11) | 0.0221 (11) | 0.0204 (10) | 0.0099 (9) | 0.0020 (9) | −0.0010 (9) |
| O2 | 0.0280 (11) | 0.0260 (11) | 0.0175 (11) | 0.0092 (9) | 0.0041 (9) | −0.0025 (9) |
| C1 | 0.0131 (14) | 0.0221 (15) | 0.0157 (13) | 0.0081 (13) | −0.0014 (12) | 0.0017 (12) |

*Geometric parameters (Å, °)*

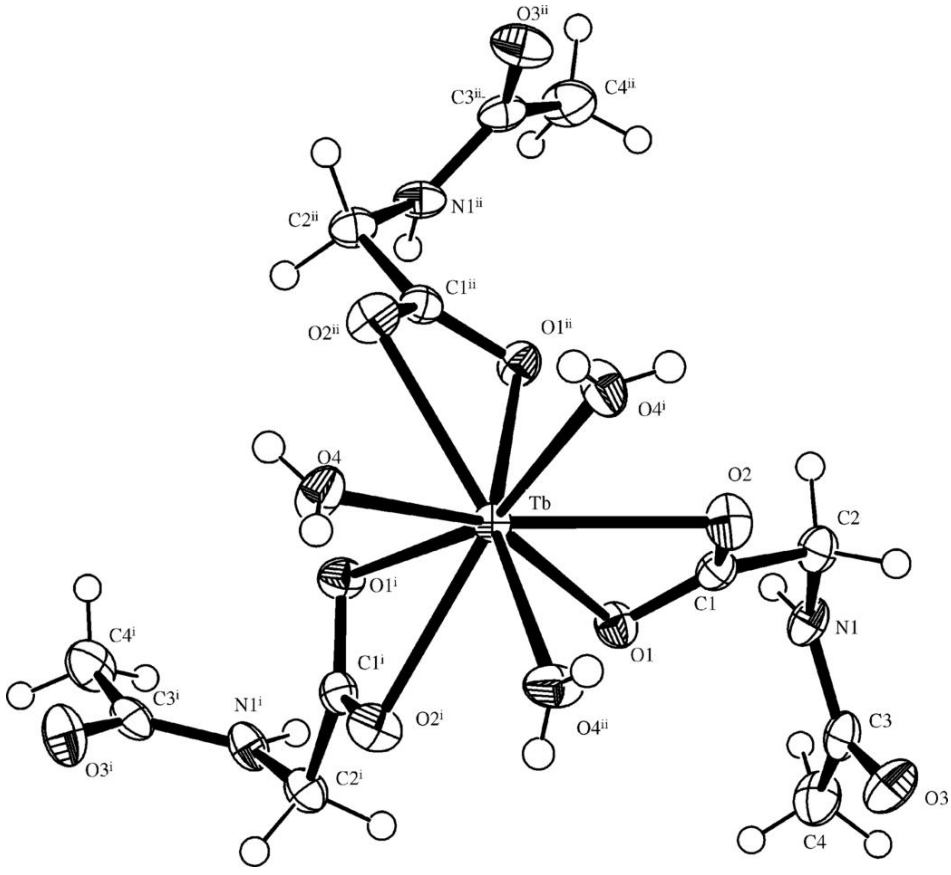
| | | | |
|---|---|---|---|
| C2—N2 | 1.445 (4) | Tb1—O4$^{i}$ | 2.359 (3) |
| C2—C1 | 1.509 (4) | Tb1—O4$^{ii}$ | 2.359 (3) |
| C2—H2B | 1.00 (4) | Tb1—O2$^{i}$ | 2.473 (2) |
| C2—H2A | 0.95 (5) | Tb1—O2$^{ii}$ | 2.473 (2) |
| N2—C3 | 1.345 (4) | Tb1—O2 | 2.473 (2) |
| N2—H1 | 0.94 (5) | Tb1—O1$^{i}$ | 2.513 (2) |
| C3—O3 | 1.239 (4) | Tb1—O1 | 2.513 (2) |
| C3—C4 | 1.492 (5) | Tb1—O1$^{ii}$ | 2.513 (2) |
| C4—H4A | 1.00 (6) | Tb1—C1$^{i}$ | 2.847 (3) |
| C4—H4C | 0.92 (7) | Tb1—C1$^{ii}$ | 2.847 (3) |
| C4—H4B | 0.94 (6) | Tb1—C1 | 2.847 (3) |
| O4—H2W | 0.934 | O1—C1 | 1.266 (4) |
| O4—H1W | 0.868 | O2—C1 | 1.258 (4) |
| Tb1—O4 | 2.359 (3) | | |
| N2—C2—C1 | 115.2 (3) | O1$^{i}$—Tb1—O1 | 73.53 (8) |
| N2—C2—H2B | 113 (2) | O4$^{i}$—Tb1—O1$^{ii}$ | 93.22 (9) |
| C1—C2—H2B | 103 (2) | O4$^{ii}$—Tb1—O1$^{ii}$ | 158.57 (8) |
| N2—C2—H2A | 113 (3) | O4—Tb1—O1$^{ii}$ | 119.55 (8) |
| C1—C2—H2A | 103 (3) | O2$^{i}$—Tb1—O1$^{ii}$ | 123.70 (7) |
| H2B—C2—H2A | 109 (4) | O2$^{ii}$—Tb1—O1$^{ii}$ | 51.97 (7) |
| C3—N2—C2 | 121.0 (3) | O2—Tb1—O1$^{ii}$ | 78.21 (8) |
| C3—N2—H1 | 119 (3) | O1$^{i}$—Tb1—O1$^{ii}$ | 73.53 (8) |
| C2—N2—H1 | 120 (3) | O1—Tb1—O1$^{ii}$ | 73.53 (8) |
| O3—C3—N2 | 120.6 (3) | O4$^{i}$—Tb1—C1$^{i}$ | 167.21 (8) |
| O3—C3—C4 | 122.4 (3) | O4$^{ii}$—Tb1—C1$^{i}$ | 93.26 (10) |
| N2—C3—C4 | 117.1 (3) | O4—Tb1—C1$^{i}$ | 90.32 (11) |
| C3—C4—H4A | 113 (3) | O2$^{i}$—Tb1—C1$^{i}$ | 26.15 (8) |
| C3—C4—H4C | 111 (4) | O2$^{ii}$—Tb1—C1$^{i}$ | 101.31 (9) |
| H4A—C4—H4C | 109 (5) | O2—Tb1—C1$^{i}$ | 121.02 (9) |
| C3—C4—H4B | 115 (4) | O1$^{i}$—Tb1—C1$^{i}$ | 26.40 (8) |
| H4A—C4—H4B | 102 (5) | O1—Tb1—C1$^{i}$ | 70.24 (9) |
| H4C—C4—H4B | 106 (5) | O1$^{ii}$—Tb1—C1$^{i}$ | 97.76 (8) |
| Tb1—O4—H2W | 122.7 | O4$^{i}$—Tb1—C1$^{ii}$ | 90.32 (11) |
| Tb1—O4—H1W | 105.44 | O4$^{ii}$—Tb1—C1$^{ii}$ | 167.21 (8) |
| H2W—O4—H1W | 131.8 | O4—Tb1—C1$^{ii}$ | 93.26 (10) |
| O4$^{i}$—Tb1—O4$^{ii}$ | 78.52 (11) | O2$^{i}$—Tb1—C1$^{ii}$ | 121.02 (9) |
| O4$^{i}$—Tb1—O4 | 78.52 (11) | O2$^{ii}$—Tb1—C1$^{ii}$ | 26.15 (8) |
| O4$^{ii}$—Tb1—O4 | 78.52 (11) | O2—Tb1—C1$^{ii}$ | 101.31 (9) |
| O4$^{i}$—Tb1—O2$^{i}$ | 142.98 (9) | O1$^{i}$—Tb1—C1$^{ii}$ | 70.24 (9) |

| | | | |
|---|---|---|---|
| O4$^{ii}$—Tb1—O2$^{i}$ | 67.66 (8) | O1—Tb1—C1$^{ii}$ | 97.76 (8) |
| O4—Tb1—O2$^{i}$ | 80.36 (9) | O1$^{ii}$—Tb1—C1$^{ii}$ | 26.40 (8) |
| O4$^{i}$—Tb1—O2$^{ii}$ | 80.36 (9) | C1$^{i}$—Tb1—C1$^{ii}$ | 96.60 (9) |
| O4$^{ii}$—Tb1—O2$^{ii}$ | 142.98 (9) | O4$^{i}$—Tb1—C1 | 93.26 (10) |
| O4—Tb1—O2$^{ii}$ | 67.66 (8) | O4$^{ii}$—Tb1—C1 | 90.32 (11) |
| O2$^{i}$—Tb1—O2$^{ii}$ | 118.52 (2) | O4—Tb1—C1 | 167.21 (8) |
| O4$^{i}$—Tb1—O2 | 67.66 (8) | O2$^{i}$—Tb1—C1 | 101.31 (9) |
| O4$^{ii}$—Tb1—O2 | 80.36 (9) | O2$^{ii}$—Tb1—C1 | 121.02 (9) |
| O4—Tb1—O2 | 142.98 (9) | O2—Tb1—C1 | 26.15 (8) |
| O2$^{i}$—Tb1—O2 | 118.52 (2) | O1$^{i}$—Tb1—C1 | 97.76 (8) |
| O2$^{ii}$—Tb1—O2 | 118.52 (2) | O1—Tb1—C1 | 26.40 (8) |
| O4$^{i}$—Tb1—O1$^{i}$ | 158.57 (8) | O1$^{ii}$—Tb1—C1 | 70.24 (9) |
| O4$^{ii}$—Tb1—O1$^{i}$ | 119.55 (8) | C1$^{i}$—Tb1—C1 | 96.60 (9) |
| O4—Tb1—O1$^{i}$ | 93.22 (9) | C1$^{ii}$—Tb1—C1 | 96.60 (9) |
| O2$^{i}$—Tb1—O1$^{i}$ | 51.97 (7) | C1—O1—Tb1 | 91.7 (2) |
| O2$^{ii}$—Tb1—O1$^{i}$ | 78.21 (8) | C1—O2—Tb1 | 93.8 (2) |
| O2—Tb1—O1$^{i}$ | 123.70 (8) | O2—C1—O1 | 119.9 (3) |
| O4$^{i}$—Tb1—O1 | 119.55 (8) | O2—C1—C2 | 117.5 (3) |
| O4$^{ii}$—Tb1—O1 | 93.22 (9) | O1—C1—C2 | 122.3 (3) |
| O4—Tb1—O1 | 158.57 (8) | O2—C1—Tb1 | 60.08 (17) |
| O2$^{i}$—Tb1—O1 | 78.21 (8) | O1—C1—Tb1 | 61.90 (18) |
| O2$^{ii}$—Tb1—O1 | 123.70 (7) | C2—C1—Tb1 | 159.6 (2) |
| O2—Tb1—O1 | 51.97 (7) | | |
| C1—C2—N2—C3 | −77.5 (4) | O4$^{ii}$—Tb1—C1—O2 | −67.0 (2) |
| C2—N2—C3—O3 | −4.4 (5) | O4—Tb1—C1—O2 | −37.9 (5) |
| C2—N2—C3—C4 | 173.7 (3) | O2$^{i}$—Tb1—C1—O2 | −134.22 (18) |
| O4$^{i}$—Tb1—O1—C1 | −5.6 (3) | O2$^{ii}$—Tb1—C1—O2 | 92.27 (16) |
| O4$^{ii}$—Tb1—O1—C1 | −84.2 (2) | O1$^{i}$—Tb1—C1—O2 | 173.14 (19) |
| O4—Tb1—O1—C1 | −150.5 (2) | O1—Tb1—C1—O2 | −163.6 (3) |
| O2$^{i}$—Tb1—O1—C1 | −150.6 (2) | O1$^{ii}$—Tb1—C1—O2 | 103.8 (2) |
| O2$^{ii}$—Tb1—O1—C1 | 92.8 (2) | C1$^{i}$—Tb1—C1—O2 | −160.3 (2) |
| O2—Tb1—O1—C1 | −9.12 (19) | C1$^{ii}$—Tb1—C1—O2 | 102.3 (2) |
| O1$^{i}$—Tb1—O1—C1 | 155.9 (2) | O4$^{i}$—Tb1—C1—O1 | 175.1 (2) |
| O1$^{ii}$—Tb1—O1—C1 | 78.6 (2) | O4$^{ii}$—Tb1—C1—O1 | 96.60 (19) |
| C1$^{i}$—Tb1—O1—C1 | −176.5 (2) | O4—Tb1—C1—O1 | 125.6 (4) |
| C1$^{ii}$—Tb1—O1—C1 | 89.20 (15) | O2$^{i}$—Tb1—C1—O1 | 29.3 (2) |
| O4$^{i}$—Tb1—O2—C1 | −167.5 (2) | O2$^{ii}$—Tb1—C1—O1 | −104.2 (2) |
| O4$^{ii}$—Tb1—O2—C1 | 111.0 (2) | O2—Tb1—C1—O1 | 163.6 (3) |
| O4—Tb1—O2—C1 | 166.95 (19) | O1$^{i}$—Tb1—C1—O1 | −23.3 (2) |
| O2$^{i}$—Tb1—O2—C1 | 53.1 (2) | O1$^{ii}$—Tb1—C1—O1 | −92.6 (2) |
| O2$^{ii}$—Tb1—O2—C1 | −102.93 (19) | C1$^{i}$—Tb1—C1—O1 | 3.3 (2) |

| | | | |
|---|---|---|---|
| O1$^{i}$—Tb1—O2—C1 | −8.2 (2) | C1$^{ii}$—Tb1—C1—O1 | −94.18 (15) |
| O1—Tb1—O2—C1 | 9.20 (19) | O4$^{i}$—Tb1—C1—C2 | −77.4 (6) |
| O1$^{ii}$—Tb1—O2—C1 | −69.0 (2) | O4$^{ii}$—Tb1—C1—C2 | −155.9 (6) |
| C1$^{i}$—Tb1—O2—C1 | 23.0 (2) | O4—Tb1—C1—C2 | −126.9 (6) |
| C1$^{ii}$—Tb1—O2—C1 | −81.9 (2) | O2$^{i}$—Tb1—C1—C2 | 136.8 (6) |
| Tb1—O2—C1—O1 | −16.7 (4) | O2$^{ii}$—Tb1—C1—C2 | 3.3 (7) |
| Tb1—O2—C1—C2 | 156.9 (3) | O2—Tb1—C1—C2 | −88.9 (7) |
| Tb1—O1—C1—O2 | 16.4 (3) | O1$^{i}$—Tb1—C1—C2 | 84.2 (6) |
| Tb1—O1—C1—C2 | −156.8 (3) | O1—Tb1—C1—C2 | 107.5 (7) |
| N2—C2—C1—O2 | 168.9 (3) | O1$^{ii}$—Tb1—C1—C2 | 14.9 (6) |
| N2—C2—C1—O1 | −17.6 (5) | C1$^{i}$—Tb1—C1—C2 | 110.8 (6) |
| N2—C2—C1—Tb1 | −113.4 (6) | C1$^{ii}$—Tb1—C1—C2 | 13.3 (7) |
| O4$^{i}$—Tb1—C1—O2 | 11.56 (19) | | |

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

**Fig. 1**


O3ii
C3ii
C4ii
N1ii
C2ii
C1ii
O2ii
O1ii
O4i
O4
Tb
O2
C2
O1i
C1
N1
C4i
C1i
O1
C3i
N1i
O2i
O4ii
C3
O3i
C2i
O3
C4