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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$
 R factor = 0.027
 wR factor = 0.059
Data-to-parameter ratio = 13.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Tetra- μ -benzoato-bis[benzoato(2,2'-bipyridyl)-
terbium(III)]

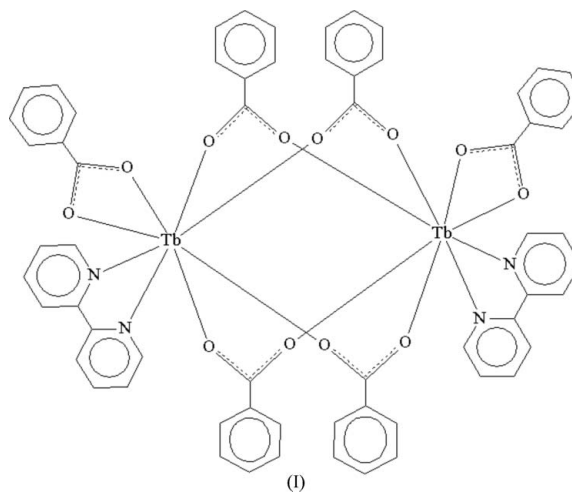
In the title compound, $[\text{Tb}_2(\text{C}_7\text{H}_5\text{O}_2)_6(\text{C}_{10}\text{H}_8\text{N}_2)_2]$, two Tb^{III} ions are linked by four carboxylate groups in bidentate bridging modes, forming a binuclear unit. Each Tb^{III} ion is eight-coordinated by one 2,2'-bipyridyl molecule, one bidentate carboxylate group and four bridging carboxylate groups, giving distorted square-antiprismatic geometry.

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Comment

Lanthanide complexes of organic ligands, especially Eu^{III} or Tb^{III} complexes, often show excellent luminescence (Guo *et al.*, 2005; Zhang *et al.*, 2005; Liu *et al.*, 2004). The choice of appropriate ligands is a key step in determining the luminescent characteristics of the complexes. Aromatic carboxylic acids are strong ligands to coordinate lanthanide metals. In this work, an efficient luminescent terbium complex with benzoate and 2,2'-bipyridyl ligands, (I), has been prepared and its structure determined.



The crystal structure of the title compound contains binuclear molecules $[\text{Tb}(\text{BA})_3(\text{bipy})]_2$. The structure is shown in Fig. 1. In each molecule, two Tb^{III} ions are linked by four carboxylate groups in a bidentate bridging mode. The intramolecular distance between the two Tb^{III} ions is 4.344 (2) Å. Each Tb^{III} ion resides in an eight-coordinate distorted square-antiprismatic environment (Fig. 2), with four of the coordination sites occupied by the O atoms of the bridging carboxylates, two by the O atoms of the terminal bidentate carboxylates, and the remaining positions occupied by two N atoms of a 2,2'-bipyridyl molecule.

The Tb—O distances are in the range 2.286 (3)–2.465 (2) Å, of which the Tb—O bonds formed by the terminal bidentate

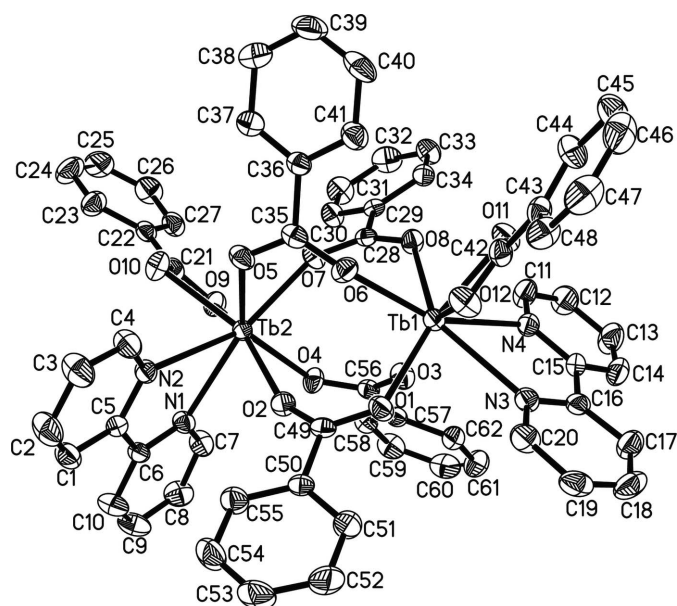


Figure 1
The molecular structure, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.

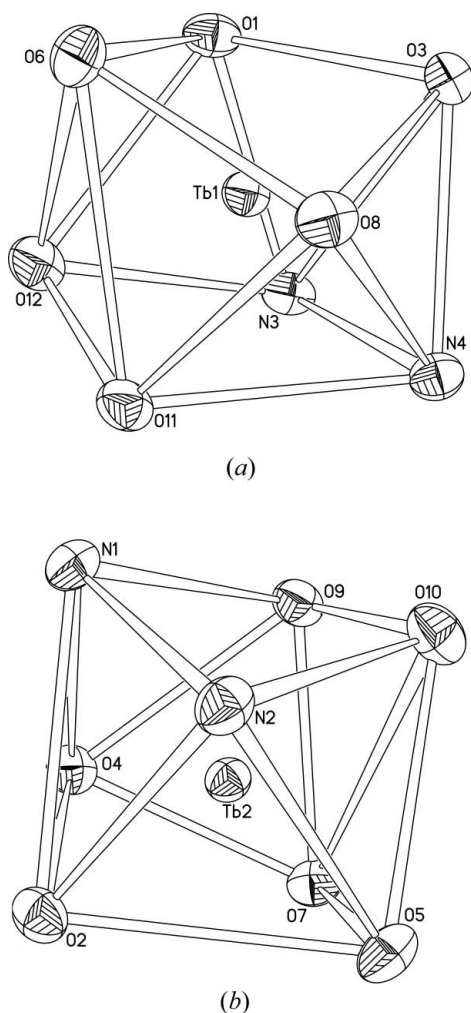


Figure 2
The coordination polyhedron of (a) the Tb1 ion and (b) the Tb2 ion.

carboxylate groups are longer [average distance = 2.435 (2) Å] than those formed by the bridging carboxylates [average distance = 2.322 (2) Å]. The Tb—N distances are in the range 2.552 (3)–2.621 (3) Å. The five-membered chelate ring containing two N atoms and the terbium ion is nearly coplanar with the 2,2′-bipyridyl molecule [dihedral angle = 2.7 (1) or 5.1 (1)°].

Experimental

Stoichiometric amounts of terbium chloride, benzoic acid and 1,10-phenanthroline were dissolved separately in 95% ethanol. The pH value of the benzoic acid was adjusted to the range 6–7 with NaOH solution. The solutions of the two ligands were mixed and the mixture was added dropwise to the ethanolic TbCl₃ solution; a white precipitate then formed. The mixture was stirred for 4 h and then filtered. The filtrate was slowly evaporated at room temperature, and colourless crystals suitable for X-ray investigation were obtained. Analysis calculated for C₆₂H₄₆N₄O₁₂Tb₂: C 54.88, H 3.42, N 4.13%; found: C 54.12, H 3.29, N 3.89%.

Crystal data

[Tb₂(C₇H₅O₂)₆(C₁₀H₈N₂)₂]
M_r = 1356.87
 Monoclinic, *P*2₁/*n*
a = 14.1379 (9) Å
b = 15.3995 (10) Å
c = 25.9625 (16) Å
 β = 103.435 (1)°
V = 5497.8 (6) Å³

Z = 4
D_x = 1.639 Mg m⁻³
 Mo *K*α radiation
 μ = 2.62 mm⁻¹
T = 293 (2) K
 Block, colourless
 0.32 × 0.16 × 0.10 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.781, *T_{max}* = 1.000
 (expected range = 0.601–0.770)

29568 measured reflections
 9710 independent reflections
 7548 reflections with *I* > 2σ(*I*)
R_{int} = 0.037
 θ_{\max} = 25.0°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.027
wR (*F*²) = 0.059
S = 1.04
 9710 reflections
 721 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.019P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 0.44 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.47 \text{ e \AA}^{-3}$

H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding on their parent atoms, with *U_{iso}*(H) = 1.2*U_{eq}*(C).

Data collection: SMART-NT (Bruker, 1998); cell refinement: SMART-NT; data reduction: SAINT-NT (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-NT (Bruker, 1998); software used to prepare material for publication: SHELXTL-NT.

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