

Bis(2,2'-bipyridine)-1 κ^2 N,N';3 κ^2 N,N'-hexa- μ -methacrylate-1:2 κ^6 O:O';-2:3 κ^6 O:O'-(nitrate-2 κ^2 O,O')-1,3-dicobalt(II)-2-terbium(III)

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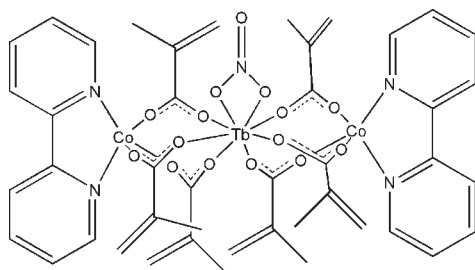
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.025; wR factor = 0.060; data-to-parameter ratio = 13.2.

In the title trinuclear cobalt–terbium complex, $[\text{Co}_2\text{Tb}(\text{C}_4\text{H}_5\text{O}_2)_6(\text{NO}_3)(\text{C}_{10}\text{H}_8\text{N}_2)_2]$, the central Tb^{III} and each of the Co^{II} ions are bridged by three carboxylate groups of the methacrylate anions. The Tb^{III} cation is coordinated by six O atoms from six methacrylate anions and two O atoms from a chelating nitrate anion in a distorted square-antiprismatic geometry. Each Co^{II} ion is coordinated by three O atoms from three methacrylate anions and two N atoms of a 2,2'-bipyridine ligand in a distorted square-pyramidal geometry. In the crystal structure, π - π stacking between the pyridine rings [centroid–centroid distances = 3.682 (8) and 3.760 (8) Å] is observed and weak intermolecular C–H \cdots O hydrogen bonding is also present.

Related literature

For the crystal structures of analogous complexes, see: Wu & Guo (2004); Zhu *et al.* (2005); Wu (2008); Wu & Hou (2010). For details of the preparation of $\text{TbL}_3\cdot\text{H}_2\text{O}$ (HL = $\text{CH}_2\text{C}(\text{CH}_3)\text{COOH}$), see: Lu *et al.* (1995).



Experimental

Crystal data

| | |
|--|-----------------------------------|
| $[\text{Co}_2\text{Tb}(\text{C}_4\text{H}_5\text{O}_2)_6(\text{NO}_3)(\text{C}_{10}\text{H}_8\text{N}_2)_2]$ | $\beta = 99.950$ (2) $^\circ$ |
| $M_r = 1161.64$ | $\gamma = 99.845$ (3) $^\circ$ |
| Triclinic, $P\bar{1}$ | $V = 2330.26$ (19) Å ³ |
| $a = 11.3717$ (6) Å | $Z = 2$ |
| $b = 13.4396$ (5) Å | Mo $K\alpha$ radiation |
| $c = 16.3572$ (8) Å | $\mu = 2.28$ mm ⁻¹ |
| $\alpha = 103.912$ (2) $^\circ$ | $T = 293$ K |
| | $0.32 \times 0.31 \times 0.15$ mm |

Data collection

| | |
|---|--|
| Rigaku R-Axis RAPID diffractometer | 13172 measured reflections |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | 8051 independent reflections |
| $T_{\min} = 0.495$, $T_{\max} = 0.709$ | 7272 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.031$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.025$ | 610 parameters |
| $wR(F^2) = 0.060$ | H-atom parameters constrained |
| $S = 1.03$ | $\Delta\rho_{\max} = 0.45$ e Å ⁻³ |
| 8051 reflections | $\Delta\rho_{\min} = -0.87$ e Å ⁻³ |

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|-------|-------------|-------------|---------------|
| C8–H8 \cdots O9 ⁱ | 0.93 | 2.46 | 3.299 (4) | 150 |
| C9–H9 \cdots O7 ⁱ | 0.93 | 2.54 | 3.291 (4) | 138 |
| C38–H38 \cdots O11 ⁱⁱ | 0.93 | 2.58 | 3.457 (4) | 157 |
| C42–H42 \cdots O9 ⁱⁱⁱ | 0.93 | 2.42 | 3.259 (5) | 150 |
| C43–H43 \cdots O8 ⁱⁱⁱ | 0.93 | 2.57 | 3.316 (4) | 138 |

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5010).

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Acta Cryst. (2010). E66, m1075 [doi:10.1107/S1600536810031053]

Bis(2,2'-bipyridine)-1 κ^2 N,N';3 κ^2 N,N'-hexa- μ -methacrylato-1:2 κ^6 O:O';2:3 κ^6 O:O'-(nitrate-2 κ^2 O,O')-1,3-dicobalt(II)-2-terbium(III)

B. Wu and C.-X. Zhao

Comment

The study of heterometallic complexes containing d-transition metal and lanthanide(III) cations connected by bridging ligands is being actively pursued because of their relevance in solid-state technology and as models for magnetic studies. As a contribution to a structural study of heterometallic complexes containing d-transition metal and rare-earth(III) cations (Wu & Guo, 2004; Zhu *et al.*, 2005; Wu, 2008), herewith we report the synthesis and crystal structure of the title compound, (I).

The crystal structure of the title Co—Tb—Co trinuclear complex is similar to the known crystal structures of the Zn—Ce—Zn, Zn—Nd—Zn, Co—Gd—Co and Co—Ce—Co complexes (Wu & Guo, 2004; Zhu *et al.*, 2005; Wu, 2008; Wu & Hou, 2010). The Tb^{III} center is coordinated by six O atoms from six methacrylato ligands and two O atoms from nitrate anion in a distorted square-antiprismatic geometry. Each Co^{II} ion is coordinated by three O atoms from three methacrylato ligands and two N atoms from 2,2'-bipyridine ligand in a distorted pyramidal geometry. The Tb^{III} and each of two Co^{II} ions are bridged by three bidentate methacrylato ligands. Two Tb \cdots Co separations are almost equal. The separations of Tb \cdots Co1 and Tb \cdots Co2 are 3.937 (1) and 3.822 (1) Å, respectively.

In the crystal structure, π - π interactions between the aromatic rings [centroid-centroid distances of 3.682 (8) and 3.760 (8) Å, respectively] link molecules into chains propagated in direction [01-1]. The aromatic stacking interactions are responsible for the supramolecular assemblies. Weak intermolecular C—H \cdots O hydrogen bonds stabilize further the crystal packing (Table 1).

Experimental

TbL₃.H₂O (864 mg, 2.0 mmol; HL = CH₂C(CH₃)COOH) and Co(NO₃)₂.6H₂O (435 mg, 1.5 mmol) were dissolved in 15 ml water, and the pH adjusted to 4.0 using HL. An ethanol solution (3 ml) of 2,2'-bipyridine (234 mg, 1.5 mmol) was added into the above solution with stirring. After filtration, the filtrate was allowed to stand at room temperature and single crystals suitable for X-ray work were obtained after two weeks.

Refinement

H atoms were placed in idealized locations with C—H distances 0.93 - 0.96 Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C).

Figures



Fig. 1. View of the molecule showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. All H atoms have been omitted for clarity.

Bis(2,2'-bipyridine)-1 κ^2 N,N';3 κ^2 N,N'-hexa- μ -methacrylate-1:2 κ^6 O:O';2:3 κ^6 O:O'-(nitrate-2 κ^2 O,O')-1,3-dicobalt(II)-2-terbium(III)

Crystal data

[Co₂Tb(C₄H₅O₂)₆(NO₃)(C₁₀H₈N₂)₂]

$M_r = 1161.64$

Triclinic, *PT*

Hall symbol: -P 1

$a = 11.3717$ (6) Å

$b = 13.4396$ (5) Å

$c = 16.3572$ (8) Å

$\alpha = 103.912$ (2)°

$\beta = 99.950$ (2)°

$\gamma = 99.845$ (3)°

$V = 2330.26$ (19) Å³

$Z = 2$

$F(000) = 1168$

$D_x = 1.656$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 10681 reflections

$\theta = 2.0$ – 27.5 °

$\mu = 2.28$ mm⁻¹

$T = 293$ K

Block, brown

$0.32 \times 0.31 \times 0.15$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: 10.00 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.495$, $T_{\max} = 0.709$

13172 measured reflections

8051 independent reflections

7272 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 25.1$ °, $\theta_{\min} = 1.3$ °

$h = -13$ → 13

$k = -16$ → 16

$l = -19$ → 19

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.060$

$S = 1.03$

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

$w = 1/[\sigma^2(F_o^2) + (0.0316P)^2 + 2.6217P]$

8051 reflections
610 parameters
0 restraints

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.45 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.87 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|--------------|----------------------------------|
| Tb | 0.349851 (12) | 0.235738 (10) | 0.240894 (8) | 0.01582 (5) |
| Co1 | 0.28569 (3) | 0.09556 (3) | 0.41926 (2) | 0.01591 (9) |
| Co2 | 0.28401 (3) | 0.42261 (3) | 0.10445 (2) | 0.01763 (9) |
| O1 | 0.45584 (18) | 0.17936 (16) | 0.47967 (13) | 0.0221 (4) |
| O2 | 0.47217 (19) | 0.26143 (17) | 0.37769 (13) | 0.0268 (5) |
| O3 | 0.19771 (19) | 0.21432 (16) | 0.45824 (14) | 0.0253 (5) |
| O4 | 0.2203 (2) | 0.2614 (3) | 0.33945 (16) | 0.0486 (7) |
| O5 | 0.33886 (19) | -0.01681 (16) | 0.33430 (13) | 0.0237 (5) |
| O6 | 0.2821 (2) | 0.06055 (17) | 0.23263 (16) | 0.0308 (5) |
| O7 | 0.5251 (2) | 0.14495 (17) | 0.22325 (14) | 0.0272 (5) |
| O8 | 0.56465 (19) | 0.31214 (17) | 0.23419 (14) | 0.0253 (5) |
| O9 | 0.7096 (2) | 0.2241 (2) | 0.22484 (17) | 0.0405 (6) |
| O10 | 0.15112 (19) | 0.22751 (18) | 0.16450 (14) | 0.0270 (5) |
| O11 | 0.13244 (19) | 0.30122 (16) | 0.05503 (14) | 0.0243 (5) |
| O12 | 0.35412 (19) | 0.19272 (17) | 0.09420 (13) | 0.0255 (5) |
| O13 | 0.38403 (19) | 0.33206 (16) | 0.04124 (13) | 0.0235 (4) |
| O14 | 0.36667 (18) | 0.41464 (16) | 0.24671 (13) | 0.0229 (4) |
| O15 | 0.43760 (19) | 0.53596 (16) | 0.18666 (13) | 0.0253 (5) |
| N1 | 0.1041 (2) | -0.00293 (19) | 0.36608 (15) | 0.0189 (5) |
| N2 | 0.2646 (2) | 0.01087 (18) | 0.50865 (15) | 0.0173 (5) |
| N3 | 0.6023 (2) | 0.2265 (2) | 0.22695 (17) | 0.0263 (6) |
| N4 | 0.1622 (2) | 0.5164 (2) | 0.14918 (16) | 0.0225 (5) |
| N5 | 0.2614 (2) | 0.50765 (19) | 0.01371 (16) | 0.0208 (5) |
| C1 | 0.0287 (3) | -0.0066 (2) | 0.29172 (19) | 0.0235 (6) |
| H1 | 0.0560 | 0.0359 | 0.2585 | 0.028* |
| C2 | -0.0880 (3) | -0.0713 (3) | 0.2625 (2) | 0.0263 (7) |
| H2 | -0.1375 | -0.0727 | 0.2104 | 0.032* |
| C3 | -0.1289 (3) | -0.1337 (2) | 0.31281 (19) | 0.0234 (6) |

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|------|-------------|-------------|--------------|------------|
| H3 | -0.2066 | -0.1778 | 0.2950 | 0.028* |
| C4 | -0.0520 (3) | -0.1294 (2) | 0.39046 (19) | 0.0215 (6) |
| H4 | -0.0783 | -0.1698 | 0.4255 | 0.026* |
| C5 | 0.0650 (3) | -0.0639 (2) | 0.41511 (18) | 0.0183 (6) |
| C6 | 0.1558 (3) | -0.0565 (2) | 0.49490 (18) | 0.0180 (6) |
| C7 | 0.1328 (3) | -0.1151 (2) | 0.55283 (19) | 0.0221 (6) |
| H7 | 0.0568 | -0.1598 | 0.5438 | 0.027* |
| C8 | 0.2248 (3) | -0.1057 (2) | 0.6238 (2) | 0.0262 (7) |
| H8 | 0.2109 | -0.1443 | 0.6627 | 0.031* |
| C9 | 0.3378 (3) | -0.0386 (2) | 0.6366 (2) | 0.0248 (7) |
| H9 | 0.4009 | -0.0320 | 0.6834 | 0.030* |
| C10 | 0.3538 (3) | 0.0187 (2) | 0.57728 (19) | 0.0226 (6) |
| H10 | 0.4291 | 0.0640 | 0.5853 | 0.027* |
| C11 | 0.5147 (3) | 0.2422 (2) | 0.44716 (18) | 0.0184 (6) |
| C12 | 0.6439 (3) | 0.2969 (2) | 0.4958 (2) | 0.0235 (6) |
| C13 | 0.6891 (3) | 0.2726 (3) | 0.5778 (2) | 0.0353 (8) |
| H13A | 0.7746 | 0.3050 | 0.5992 | 0.053* |
| H13B | 0.6776 | 0.1978 | 0.5676 | 0.053* |
| H13C | 0.6443 | 0.2992 | 0.6196 | 0.053* |
| C14 | 0.7116 (3) | 0.3622 (3) | 0.4627 (3) | 0.0372 (8) |
| H14A | 0.7919 | 0.3953 | 0.4915 | 0.045* |
| H14B | 0.6783 | 0.3745 | 0.4109 | 0.045* |
| C15 | 0.1775 (3) | 0.2680 (2) | 0.40533 (18) | 0.0217 (6) |
| C16 | 0.0906 (3) | 0.3387 (2) | 0.4226 (2) | 0.0232 (6) |
| C17 | 0.0866 (3) | 0.3841 (2) | 0.5151 (2) | 0.0293 (7) |
| H17A | 0.0281 | 0.4279 | 0.5176 | 0.044* |
| H17B | 0.1661 | 0.4254 | 0.5467 | 0.044* |
| H17C | 0.0631 | 0.3282 | 0.5401 | 0.044* |
| C18 | 0.0152 (4) | 0.3511 (3) | 0.3553 (3) | 0.0415 (9) |
| H18A | 0.0174 | 0.3163 | 0.2993 | 0.050* |
| H18B | -0.0394 | 0.3946 | 0.3644 | 0.050* |
| C19 | 0.3180 (2) | -0.0150 (2) | 0.2567 (2) | 0.0206 (6) |
| C20 | 0.3335 (3) | -0.1085 (2) | 0.19035 (19) | 0.0209 (6) |
| C21 | 0.3480 (3) | -0.2036 (2) | 0.2209 (2) | 0.0299 (7) |
| H21A | 0.3576 | -0.2581 | 0.1740 | 0.045* |
| H21B | 0.2767 | -0.2282 | 0.2406 | 0.045* |
| H21C | 0.4190 | -0.1853 | 0.2674 | 0.045* |
| C22 | 0.3347 (3) | -0.1025 (3) | 0.1107 (2) | 0.0348 (8) |
| H22A | 0.3449 | -0.1595 | 0.0695 | 0.042* |
| H22B | 0.3252 | -0.0411 | 0.0960 | 0.042* |
| C23 | 0.0991 (3) | 0.2310 (2) | 0.09099 (19) | 0.0219 (6) |
| C24 | -0.0130 (3) | 0.1450 (2) | 0.0413 (2) | 0.0246 (7) |
| C25 | -0.0923 (3) | 0.1017 (3) | 0.0924 (3) | 0.0394 (9) |
| H25A | -0.1544 | 0.0431 | 0.0550 | 0.059* |
| H25B | -0.1304 | 0.1549 | 0.1200 | 0.059* |
| H25C | -0.0440 | 0.0788 | 0.1355 | 0.059* |
| C26 | -0.0316 (3) | 0.1097 (3) | -0.0457 (2) | 0.0336 (8) |
| H26A | -0.0978 | 0.0549 | -0.0767 | 0.040* |
| H26B | 0.0217 | 0.1402 | -0.0745 | 0.040* |

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|------|-------------|------------|---------------|------------|
| C27 | 0.3746 (3) | 0.2350 (2) | 0.03536 (19) | 0.0215 (6) |
| C28 | 0.3872 (3) | 0.1660 (2) | -0.04942 (19) | 0.0227 (6) |
| C29 | 0.3929 (3) | 0.0663 (3) | -0.0578 (2) | 0.0327 (8) |
| H29A | 0.4009 | 0.0247 | -0.1100 | 0.039* |
| H29B | 0.3888 | 0.0381 | -0.0115 | 0.039* |
| C30 | 0.3930 (3) | 0.2180 (3) | -0.1208 (2) | 0.0328 (8) |
| H30A | 0.3975 | 0.1674 | -0.1721 | 0.049* |
| H30B | 0.4643 | 0.2745 | -0.1038 | 0.049* |
| H30C | 0.3210 | 0.2452 | -0.1321 | 0.049* |
| C31 | 0.4425 (3) | 0.5002 (2) | 0.25101 (19) | 0.0206 (6) |
| C32 | 0.5337 (3) | 0.5618 (2) | 0.33372 (19) | 0.0216 (6) |
| C33 | 0.5287 (3) | 0.5358 (3) | 0.4066 (2) | 0.0303 (7) |
| H33A | 0.5833 | 0.5756 | 0.4579 | 0.036* |
| H33B | 0.4707 | 0.4778 | 0.4064 | 0.036* |
| C34 | 0.6245 (3) | 0.6542 (3) | 0.3283 (2) | 0.0351 (8) |
| H34A | 0.6748 | 0.6901 | 0.3847 | 0.053* |
| H34B | 0.5814 | 0.7014 | 0.3067 | 0.053* |
| H34C | 0.6751 | 0.6299 | 0.2899 | 0.053* |
| C35 | 0.1151 (3) | 0.5158 (3) | 0.2190 (2) | 0.0286 (7) |
| H35 | 0.1427 | 0.4767 | 0.2551 | 0.034* |
| C36 | 0.0271 (3) | 0.5709 (3) | 0.2390 (2) | 0.0364 (8) |
| H36 | -0.0031 | 0.5698 | 0.2882 | 0.044* |
| C37 | -0.0150 (3) | 0.6276 (3) | 0.1847 (2) | 0.0353 (8) |
| H37 | -0.0749 | 0.6647 | 0.1967 | 0.042* |
| C38 | 0.0321 (3) | 0.6291 (2) | 0.1125 (2) | 0.0282 (7) |
| H38 | 0.0045 | 0.6670 | 0.0753 | 0.034* |
| C39 | 0.1215 (3) | 0.5727 (2) | 0.09632 (19) | 0.0221 (6) |
| C40 | 0.1818 (3) | 0.5716 (2) | 0.02266 (19) | 0.0215 (6) |
| C41 | 0.1620 (3) | 0.6338 (3) | -0.0332 (2) | 0.0308 (7) |
| H41 | 0.1064 | 0.6769 | -0.0268 | 0.037* |
| C42 | 0.2259 (3) | 0.6308 (3) | -0.0981 (2) | 0.0362 (8) |
| H42 | 0.2129 | 0.6711 | -0.1363 | 0.043* |
| C43 | 0.3096 (3) | 0.5670 (3) | -0.1056 (2) | 0.0328 (8) |
| H43 | 0.3549 | 0.5651 | -0.1479 | 0.039* |
| C44 | 0.3244 (3) | 0.5060 (3) | -0.0484 (2) | 0.0267 (7) |
| H44 | 0.3799 | 0.4627 | -0.0535 | 0.032* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Tb | 0.01728 (8) | 0.01693 (8) | 0.01758 (8) | 0.00519 (5) | 0.00563 (5) | 0.01065 (5) |
| Co1 | 0.01583 (19) | 0.01565 (19) | 0.01852 (19) | 0.00300 (15) | 0.00508 (15) | 0.00846 (15) |
| Co2 | 0.0185 (2) | 0.0171 (2) | 0.01853 (19) | 0.00386 (15) | 0.00212 (16) | 0.00884 (15) |
| O1 | 0.0193 (10) | 0.0230 (11) | 0.0249 (11) | 0.0003 (9) | 0.0041 (9) | 0.0119 (9) |
| O2 | 0.0259 (11) | 0.0333 (13) | 0.0215 (11) | 0.0032 (10) | 0.0023 (9) | 0.0127 (9) |
| O3 | 0.0244 (11) | 0.0215 (11) | 0.0310 (12) | 0.0075 (9) | 0.0049 (9) | 0.0082 (9) |
| O4 | 0.0281 (13) | 0.088 (2) | 0.0312 (14) | 0.0155 (14) | 0.0114 (11) | 0.0144 (14) |
| O5 | 0.0238 (11) | 0.0247 (11) | 0.0223 (11) | 0.0069 (9) | 0.0054 (9) | 0.0050 (9) |

supplementary materials

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|-----|-------------|-------------|-------------|--------------|--------------|-------------|
| O6 | 0.0237 (11) | 0.0229 (12) | 0.0546 (15) | 0.0070 (9) | 0.0135 (11) | 0.0227 (11) |
| O7 | 0.0278 (12) | 0.0296 (12) | 0.0331 (12) | 0.0115 (10) | 0.0109 (10) | 0.0187 (10) |
| O8 | 0.0252 (11) | 0.0279 (12) | 0.0307 (12) | 0.0072 (9) | 0.0108 (9) | 0.0186 (9) |
| O9 | 0.0241 (12) | 0.0699 (19) | 0.0515 (15) | 0.0244 (12) | 0.0213 (12) | 0.0427 (14) |
| O10 | 0.0198 (11) | 0.0374 (13) | 0.0260 (11) | 0.0060 (9) | 0.0033 (9) | 0.0144 (10) |
| O11 | 0.0226 (11) | 0.0178 (11) | 0.0316 (11) | 0.0018 (9) | 0.0011 (9) | 0.0108 (9) |
| O12 | 0.0299 (12) | 0.0320 (12) | 0.0210 (11) | 0.0125 (10) | 0.0091 (9) | 0.0128 (9) |
| O13 | 0.0245 (11) | 0.0234 (11) | 0.0260 (11) | 0.0081 (9) | 0.0072 (9) | 0.0099 (9) |
| O14 | 0.0210 (10) | 0.0177 (11) | 0.0317 (11) | 0.0051 (9) | 0.0063 (9) | 0.0093 (9) |
| O15 | 0.0273 (11) | 0.0231 (11) | 0.0255 (11) | 0.0027 (9) | 0.0005 (9) | 0.0128 (9) |
| N1 | 0.0193 (12) | 0.0189 (13) | 0.0202 (12) | 0.0039 (10) | 0.0057 (10) | 0.0079 (10) |
| N2 | 0.0173 (12) | 0.0188 (12) | 0.0186 (12) | 0.0048 (10) | 0.0057 (10) | 0.0091 (10) |
| N3 | 0.0224 (14) | 0.0377 (16) | 0.0293 (14) | 0.0118 (12) | 0.0092 (11) | 0.0227 (12) |
| N4 | 0.0224 (13) | 0.0229 (13) | 0.0218 (13) | 0.0050 (11) | 0.0020 (11) | 0.0077 (10) |
| N5 | 0.0189 (12) | 0.0223 (13) | 0.0228 (13) | 0.0031 (10) | 0.0029 (10) | 0.0116 (10) |
| C1 | 0.0220 (15) | 0.0286 (17) | 0.0229 (15) | 0.0039 (13) | 0.0067 (13) | 0.0127 (13) |
| C2 | 0.0219 (16) | 0.0348 (18) | 0.0227 (15) | 0.0051 (13) | 0.0025 (13) | 0.0113 (13) |
| C3 | 0.0195 (15) | 0.0198 (15) | 0.0269 (16) | 0.0002 (12) | 0.0048 (13) | 0.0021 (12) |
| C4 | 0.0238 (15) | 0.0168 (15) | 0.0265 (16) | 0.0045 (12) | 0.0088 (13) | 0.0085 (12) |
| C5 | 0.0220 (15) | 0.0133 (14) | 0.0214 (14) | 0.0054 (11) | 0.0075 (12) | 0.0050 (11) |
| C6 | 0.0200 (15) | 0.0163 (14) | 0.0220 (14) | 0.0085 (12) | 0.0092 (12) | 0.0071 (11) |
| C7 | 0.0249 (16) | 0.0177 (15) | 0.0281 (16) | 0.0038 (12) | 0.0101 (13) | 0.0121 (12) |
| C8 | 0.0337 (18) | 0.0255 (17) | 0.0280 (16) | 0.0108 (14) | 0.0094 (14) | 0.0184 (13) |
| C9 | 0.0275 (16) | 0.0280 (17) | 0.0232 (15) | 0.0124 (13) | 0.0040 (13) | 0.0123 (13) |
| C10 | 0.0197 (15) | 0.0238 (16) | 0.0274 (16) | 0.0062 (12) | 0.0047 (13) | 0.0124 (13) |
| C11 | 0.0195 (14) | 0.0166 (14) | 0.0191 (14) | 0.0061 (11) | 0.0055 (12) | 0.0026 (11) |
| C12 | 0.0187 (15) | 0.0205 (15) | 0.0276 (16) | 0.0026 (12) | 0.0027 (13) | 0.0029 (12) |
| C13 | 0.0255 (17) | 0.047 (2) | 0.0315 (18) | 0.0077 (15) | −0.0025 (15) | 0.0140 (16) |
| C14 | 0.0226 (17) | 0.036 (2) | 0.053 (2) | −0.0016 (15) | 0.0057 (16) | 0.0198 (17) |
| C15 | 0.0170 (14) | 0.0263 (16) | 0.0187 (15) | 0.0002 (12) | 0.0057 (12) | 0.0028 (12) |
| C16 | 0.0232 (15) | 0.0193 (15) | 0.0312 (16) | 0.0041 (12) | 0.0099 (13) | 0.0125 (13) |
| C17 | 0.0368 (18) | 0.0188 (16) | 0.0389 (18) | 0.0107 (14) | 0.0166 (15) | 0.0113 (14) |
| C18 | 0.047 (2) | 0.041 (2) | 0.045 (2) | 0.0197 (18) | 0.0093 (18) | 0.0233 (18) |
| C19 | 0.0125 (13) | 0.0190 (15) | 0.0313 (17) | −0.0016 (11) | 0.0078 (12) | 0.0105 (12) |
| C20 | 0.0158 (14) | 0.0231 (16) | 0.0223 (15) | 0.0007 (12) | 0.0048 (12) | 0.0058 (12) |
| C21 | 0.0326 (18) | 0.0189 (16) | 0.0344 (18) | 0.0053 (13) | 0.0050 (15) | 0.0028 (13) |
| C22 | 0.0280 (18) | 0.047 (2) | 0.0315 (18) | 0.0074 (16) | 0.0087 (15) | 0.0140 (16) |
| C23 | 0.0184 (15) | 0.0221 (16) | 0.0283 (16) | 0.0085 (12) | 0.0061 (13) | 0.0093 (13) |
| C24 | 0.0200 (15) | 0.0199 (16) | 0.0340 (17) | 0.0054 (12) | 0.0006 (13) | 0.0111 (13) |
| C25 | 0.0281 (18) | 0.040 (2) | 0.050 (2) | 0.0012 (16) | 0.0056 (17) | 0.0205 (18) |
| C26 | 0.0332 (18) | 0.0247 (17) | 0.0382 (19) | 0.0045 (14) | −0.0039 (15) | 0.0096 (14) |
| C27 | 0.0143 (14) | 0.0299 (17) | 0.0223 (15) | 0.0062 (12) | 0.0021 (12) | 0.0115 (13) |
| C28 | 0.0182 (15) | 0.0315 (17) | 0.0195 (15) | 0.0042 (13) | 0.0064 (12) | 0.0087 (13) |
| C29 | 0.0376 (19) | 0.0330 (19) | 0.0327 (18) | 0.0079 (15) | 0.0194 (16) | 0.0105 (15) |
| C30 | 0.0382 (19) | 0.040 (2) | 0.0220 (16) | 0.0088 (16) | 0.0088 (15) | 0.0095 (14) |
| C31 | 0.0179 (14) | 0.0176 (15) | 0.0280 (16) | 0.0079 (12) | 0.0040 (12) | 0.0077 (12) |
| C32 | 0.0224 (15) | 0.0210 (15) | 0.0230 (15) | 0.0082 (12) | 0.0038 (12) | 0.0073 (12) |
| C33 | 0.042 (2) | 0.0243 (17) | 0.0219 (16) | 0.0064 (14) | 0.0029 (14) | 0.0044 (13) |
| C34 | 0.0314 (18) | 0.034 (2) | 0.0337 (18) | −0.0055 (15) | −0.0004 (15) | 0.0124 (15) |

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|-----|-------------|-------------|-------------|-------------|--------------|--------------|
| C35 | 0.0292 (17) | 0.0303 (18) | 0.0254 (16) | 0.0033 (14) | 0.0048 (14) | 0.0094 (13) |
| C36 | 0.0314 (19) | 0.045 (2) | 0.0309 (18) | 0.0080 (16) | 0.0091 (15) | 0.0054 (16) |
| C37 | 0.0272 (18) | 0.0343 (19) | 0.040 (2) | 0.0126 (15) | 0.0056 (15) | -0.0004 (15) |
| C38 | 0.0268 (17) | 0.0203 (16) | 0.0325 (17) | 0.0050 (13) | -0.0004 (14) | 0.0032 (13) |
| C39 | 0.0179 (15) | 0.0167 (15) | 0.0259 (15) | 0.0006 (12) | -0.0041 (12) | 0.0037 (12) |
| C40 | 0.0225 (15) | 0.0148 (14) | 0.0251 (15) | 0.0008 (12) | -0.0002 (12) | 0.0079 (12) |
| C41 | 0.0335 (18) | 0.0233 (17) | 0.0366 (18) | 0.0075 (14) | -0.0008 (15) | 0.0156 (14) |
| C42 | 0.046 (2) | 0.0308 (19) | 0.0366 (19) | 0.0034 (16) | 0.0041 (16) | 0.0246 (16) |
| C43 | 0.0317 (18) | 0.038 (2) | 0.0320 (18) | 0.0003 (15) | 0.0083 (15) | 0.0210 (15) |
| C44 | 0.0255 (16) | 0.0283 (17) | 0.0282 (16) | 0.0046 (13) | 0.0057 (14) | 0.0126 (13) |

Geometric parameters (Å, °)

| | | | |
|---------|-----------|----------|-----------|
| Tb—O6 | 2.312 (2) | C13—H13A | 0.9600 |
| Tb—O2 | 2.334 (2) | C13—H13B | 0.9600 |
| Tb—O12 | 2.340 (2) | C13—H13C | 0.9600 |
| Tb—O10 | 2.356 (2) | C14—H14A | 0.9300 |
| Tb—O14 | 2.357 (2) | C14—H14B | 0.9300 |
| Tb—O4 | 2.369 (2) | C15—C16 | 1.499 (4) |
| Tb—O8 | 2.514 (2) | C16—C18 | 1.337 (5) |
| Tb—O7 | 2.530 (2) | C16—C17 | 1.501 (4) |
| Co1—O1 | 2.012 (2) | C17—H17A | 0.9600 |
| Co1—O5 | 2.042 (2) | C17—H17B | 0.9600 |
| Co1—O3 | 2.057 (2) | C17—H17C | 0.9600 |
| Co1—N2 | 2.078 (2) | C18—H18A | 0.9300 |
| Co1—N1 | 2.160 (2) | C18—H18B | 0.9300 |
| Co2—O13 | 2.029 (2) | C19—C20 | 1.509 (4) |
| Co2—O11 | 2.051 (2) | C20—C22 | 1.327 (4) |
| Co2—N5 | 2.088 (2) | C20—C21 | 1.503 (4) |
| Co2—O15 | 2.115 (2) | C21—H21A | 0.9600 |
| Co2—N4 | 2.133 (3) | C21—H21B | 0.9600 |
| Co2—O14 | 2.389 (2) | C21—H21C | 0.9600 |
| O1—C11 | 1.260 (3) | C22—H22A | 0.9300 |
| O2—C11 | 1.260 (3) | C22—H22B | 0.9300 |
| O3—C15 | 1.269 (4) | C23—C24 | 1.518 (4) |
| O4—C15 | 1.248 (4) | C24—C26 | 1.354 (5) |
| O5—C19 | 1.257 (4) | C24—C25 | 1.473 (5) |
| O6—C19 | 1.277 (4) | C25—H25A | 0.9600 |
| O7—N3 | 1.263 (3) | C25—H25B | 0.9600 |
| O8—N3 | 1.282 (3) | C25—H25C | 0.9600 |
| O9—N3 | 1.232 (3) | C26—H26A | 0.9300 |
| O10—C23 | 1.260 (4) | C26—H26B | 0.9300 |
| O11—C23 | 1.266 (4) | C27—C28 | 1.516 (4) |
| O12—C27 | 1.265 (4) | C28—C29 | 1.328 (5) |
| O13—C27 | 1.269 (4) | C28—C30 | 1.503 (4) |
| O14—C31 | 1.293 (4) | C29—H29A | 0.9300 |
| O15—C31 | 1.254 (4) | C29—H29B | 0.9300 |
| N1—C1 | 1.346 (4) | C30—H30A | 0.9600 |
| N1—C5 | 1.352 (4) | C30—H30B | 0.9600 |

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| N2—C10 | 1.347 (4) | C30—H30C | 0.9600 |
| N2—C6 | 1.350 (4) | C31—C32 | 1.508 (4) |
| N4—C35 | 1.343 (4) | C32—C33 | 1.328 (4) |
| N4—C39 | 1.352 (4) | C32—C34 | 1.503 (4) |
| N5—C44 | 1.338 (4) | C33—H33A | 0.9300 |
| N5—C40 | 1.353 (4) | C33—H33B | 0.9300 |
| C1—C2 | 1.390 (4) | C34—H34A | 0.9600 |
| C1—H1 | 0.9300 | C34—H34B | 0.9600 |
| C2—C3 | 1.389 (4) | C34—H34C | 0.9600 |
| C2—H2 | 0.9300 | C35—C36 | 1.381 (5) |
| C3—C4 | 1.395 (4) | C35—H35 | 0.9300 |
| C3—H3 | 0.9300 | C36—C37 | 1.379 (5) |
| C4—C5 | 1.396 (4) | C36—H36 | 0.9300 |
| C4—H4 | 0.9300 | C37—C38 | 1.382 (5) |
| C5—C6 | 1.489 (4) | C37—H37 | 0.9300 |
| C6—C7 | 1.401 (4) | C38—C39 | 1.393 (4) |
| C7—C8 | 1.386 (4) | C38—H38 | 0.9300 |
| C7—H7 | 0.9300 | C39—C40 | 1.484 (4) |
| C8—C9 | 1.389 (5) | C40—C41 | 1.394 (4) |
| C8—H8 | 0.9300 | C41—C42 | 1.383 (5) |
| C9—C10 | 1.392 (4) | C41—H41 | 0.9300 |
| C9—H9 | 0.9300 | C42—C43 | 1.387 (5) |
| C10—H10 | 0.9300 | C42—H42 | 0.9300 |
| C11—C12 | 1.509 (4) | C43—C44 | 1.391 (4) |
| C12—C14 | 1.341 (5) | C43—H43 | 0.9300 |
| C12—C13 | 1.483 (4) | C44—H44 | 0.9300 |
| O6—Tb—O2 | 89.72 (8) | C14—C12—C13 | 123.8 (3) |
| O6—Tb—O12 | 91.10 (8) | C14—C12—C11 | 119.2 (3) |
| O2—Tb—O12 | 141.89 (7) | C13—C12—C11 | 116.9 (3) |
| O6—Tb—O10 | 86.68 (8) | C12—C13—H13A | 109.5 |
| O2—Tb—O10 | 144.54 (7) | C12—C13—H13B | 109.5 |
| O12—Tb—O10 | 73.50 (7) | H13A—C13—H13B | 109.5 |
| O6—Tb—O14 | 165.64 (7) | C12—C13—H13C | 109.5 |
| O2—Tb—O14 | 97.02 (7) | H13A—C13—H13C | 109.5 |
| O12—Tb—O14 | 91.36 (7) | H13B—C13—H13C | 109.5 |
| O10—Tb—O14 | 80.47 (7) | C12—C14—H14A | 120.0 |
| O6—Tb—O4 | 83.07 (10) | C12—C14—H14B | 120.0 |
| O2—Tb—O4 | 73.78 (8) | H14A—C14—H14B | 120.0 |
| O12—Tb—O4 | 144.05 (8) | O4—C15—O3 | 124.3 (3) |
| O10—Tb—O4 | 70.76 (8) | O4—C15—C16 | 119.4 (3) |
| O14—Tb—O4 | 86.65 (9) | O3—C15—C16 | 116.2 (3) |
| O6—Tb—O8 | 122.83 (7) | C18—C16—C15 | 118.5 (3) |
| O2—Tb—O8 | 73.60 (7) | C18—C16—C17 | 123.8 (3) |
| O12—Tb—O8 | 74.10 (7) | C15—C16—C17 | 117.5 (3) |
| O10—Tb—O8 | 136.02 (7) | C16—C17—H17A | 109.5 |
| O14—Tb—O8 | 71.39 (7) | C16—C17—H17B | 109.5 |
| O4—Tb—O8 | 137.65 (9) | H17A—C17—H17B | 109.5 |
| O6—Tb—O7 | 71.84 (7) | C16—C17—H17C | 109.5 |
| O2—Tb—O7 | 71.68 (7) | H17A—C17—H17C | 109.5 |

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|-------------|-------------|---------------|-----------|
| O12—Tb—O7 | 72.45 (7) | H17B—C17—H17C | 109.5 |
| O10—Tb—O7 | 138.97 (7) | C16—C18—H18A | 120.0 |
| O14—Tb—O7 | 122.32 (7) | C16—C18—H18B | 120.0 |
| O4—Tb—O7 | 136.89 (8) | H18A—C18—H18B | 120.0 |
| O8—Tb—O7 | 51.00 (7) | O5—C19—O6 | 122.9 (3) |
| O1—Co1—O5 | 95.93 (8) | O5—C19—C20 | 117.3 (3) |
| O1—Co1—O3 | 96.07 (8) | O6—C19—C20 | 119.8 (3) |
| O5—Co1—O3 | 156.98 (8) | C22—C20—C21 | 124.4 (3) |
| O1—Co1—N2 | 96.20 (9) | C22—C20—C19 | 119.4 (3) |
| O5—Co1—N2 | 96.25 (9) | C21—C20—C19 | 116.2 (2) |
| O3—Co1—N2 | 101.89 (9) | C20—C21—H21A | 109.5 |
| O1—Co1—N1 | 173.49 (8) | C20—C21—H21B | 109.5 |
| O5—Co1—N1 | 84.80 (9) | H21A—C21—H21B | 109.5 |
| O3—Co1—N1 | 85.48 (9) | C20—C21—H21C | 109.5 |
| N2—Co1—N1 | 77.30 (9) | H21A—C21—H21C | 109.5 |
| O13—Co2—O11 | 89.61 (9) | H21B—C21—H21C | 109.5 |
| O13—Co2—N5 | 94.45 (9) | C20—C22—H22A | 120.0 |
| O11—Co2—N5 | 100.68 (9) | C20—C22—H22B | 120.0 |
| O13—Co2—O15 | 94.95 (9) | H22A—C22—H22B | 120.0 |
| O11—Co2—O15 | 164.39 (8) | O10—C23—O11 | 125.1 (3) |
| N5—Co2—O15 | 93.85 (9) | O10—C23—C24 | 118.0 (3) |
| O13—Co2—N4 | 170.11 (9) | O11—C23—C24 | 116.9 (3) |
| O11—Co2—N4 | 86.32 (9) | C26—C24—C25 | 123.9 (3) |
| N5—Co2—N4 | 77.49 (10) | C26—C24—C23 | 119.1 (3) |
| O15—Co2—N4 | 91.34 (9) | C25—C24—C23 | 117.0 (3) |
| O13—Co2—O14 | 97.41 (8) | C24—C25—H25A | 109.5 |
| O11—Co2—O14 | 106.35 (8) | C24—C25—H25B | 109.5 |
| N5—Co2—O14 | 150.45 (9) | H25A—C25—H25B | 109.5 |
| O15—Co2—O14 | 58.29 (7) | C24—C25—H25C | 109.5 |
| N4—Co2—O14 | 92.38 (8) | H25A—C25—H25C | 109.5 |
| C11—O1—Co1 | 121.33 (18) | H25B—C25—H25C | 109.5 |
| C11—O2—Tb | 158.9 (2) | C24—C26—H26A | 120.0 |
| C15—O3—Co1 | 115.23 (19) | C24—C26—H26B | 120.0 |
| C15—O4—Tb | 162.7 (2) | H26A—C26—H26B | 120.0 |
| C19—O5—Co1 | 116.41 (19) | O12—C27—O13 | 124.7 (3) |
| C19—O6—Tb | 141.31 (19) | O12—C27—C28 | 118.6 (3) |
| N3—O7—Tb | 95.80 (17) | O13—C27—C28 | 116.6 (3) |
| N3—O8—Tb | 96.05 (16) | C29—C28—C30 | 123.5 (3) |
| C23—O10—Tb | 138.55 (19) | C29—C28—C27 | 120.7 (3) |
| C23—O11—Co2 | 125.38 (19) | C30—C28—C27 | 115.8 (3) |
| C27—O12—Tb | 141.3 (2) | C28—C29—H29A | 120.0 |
| C27—O13—Co2 | 124.09 (18) | C28—C29—H29B | 120.0 |
| C31—O14—Tb | 143.88 (18) | H29A—C29—H29B | 120.0 |
| C31—O14—Co2 | 84.09 (17) | C28—C30—H30A | 109.5 |
| Tb—O14—Co2 | 107.30 (8) | C28—C30—H30B | 109.5 |
| C31—O15—Co2 | 97.56 (18) | H30A—C30—H30B | 109.5 |
| C1—N1—C5 | 119.0 (2) | C28—C30—H30C | 109.5 |
| C1—N1—Co1 | 126.30 (19) | H30A—C30—H30C | 109.5 |
| C5—N1—Co1 | 114.68 (19) | H30B—C30—H30C | 109.5 |

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| C10—N2—C6 | 119.5 (2) | O15—C31—O14 | 120.0 (3) |
| C10—N2—Co1 | 123.40 (19) | O15—C31—C32 | 118.6 (3) |
| C6—N2—Co1 | 117.13 (18) | O14—C31—C32 | 121.3 (3) |
| O9—N3—O7 | 121.5 (3) | C33—C32—C34 | 123.5 (3) |
| O9—N3—O8 | 121.4 (3) | C33—C32—C31 | 120.3 (3) |
| O7—N3—O8 | 117.1 (2) | C34—C32—C31 | 116.2 (3) |
| C35—N4—C39 | 118.8 (3) | C32—C33—H33A | 120.0 |
| C35—N4—Co2 | 125.8 (2) | C32—C33—H33B | 120.0 |
| C39—N4—Co2 | 115.0 (2) | H33A—C33—H33B | 120.0 |
| C44—N5—C40 | 119.4 (3) | C32—C34—H34A | 109.5 |
| C44—N5—Co2 | 124.1 (2) | C32—C34—H34B | 109.5 |
| C40—N5—Co2 | 116.35 (19) | H34A—C34—H34B | 109.5 |
| N1—C1—C2 | 122.8 (3) | C32—C34—H34C | 109.5 |
| N1—C1—H1 | 118.6 | H34A—C34—H34C | 109.5 |
| C2—C1—H1 | 118.6 | H34B—C34—H34C | 109.5 |
| C3—C2—C1 | 118.4 (3) | N4—C35—C36 | 122.4 (3) |
| C3—C2—H2 | 120.8 | N4—C35—H35 | 118.8 |
| C1—C2—H2 | 120.8 | C36—C35—H35 | 118.8 |
| C2—C3—C4 | 119.1 (3) | C37—C36—C35 | 118.7 (3) |
| C2—C3—H3 | 120.4 | C37—C36—H36 | 120.6 |
| C4—C3—H3 | 120.4 | C35—C36—H36 | 120.6 |
| C3—C4—C5 | 119.3 (3) | C36—C37—C38 | 119.7 (3) |
| C3—C4—H4 | 120.3 | C36—C37—H37 | 120.1 |
| C5—C4—H4 | 120.3 | C38—C37—H37 | 120.1 |
| N1—C5—C4 | 121.3 (3) | C37—C38—C39 | 118.8 (3) |
| N1—C5—C6 | 115.1 (2) | C37—C38—H38 | 120.6 |
| C4—C5—C6 | 123.7 (3) | C39—C38—H38 | 120.6 |
| N2—C6—C7 | 120.9 (3) | N4—C39—C38 | 121.5 (3) |
| N2—C6—C5 | 115.7 (2) | N4—C39—C40 | 115.0 (3) |
| C7—C6—C5 | 123.3 (3) | C38—C39—C40 | 123.5 (3) |
| C8—C7—C6 | 119.1 (3) | N5—C40—C41 | 121.1 (3) |
| C8—C7—H7 | 120.4 | N5—C40—C39 | 115.6 (2) |
| C6—C7—H7 | 120.4 | C41—C40—C39 | 123.3 (3) |
| C7—C8—C9 | 119.9 (3) | C42—C41—C40 | 119.4 (3) |
| C7—C8—H8 | 120.1 | C42—C41—H41 | 120.3 |
| C9—C8—H8 | 120.1 | C40—C41—H41 | 120.3 |
| C10—C9—C8 | 118.0 (3) | C43—C42—C41 | 119.3 (3) |
| C10—C9—H9 | 121.0 | C43—C42—H42 | 120.4 |
| C8—C9—H9 | 121.0 | C41—C42—H42 | 120.4 |
| N2—C10—C9 | 122.5 (3) | C42—C43—C44 | 118.6 (3) |
| N2—C10—H10 | 118.7 | C42—C43—H43 | 120.7 |
| C9—C10—H10 | 118.7 | C44—C43—H43 | 120.7 |
| O2—C11—O1 | 124.1 (3) | N5—C44—C43 | 122.2 (3) |
| O2—C11—C12 | 119.0 (3) | N5—C44—H44 | 118.9 |
| O1—C11—C12 | 116.9 (3) | C43—C44—H44 | 118.9 |

Hydrogen-bond geometry (Å, °)

| | | | | |
|-------------------------|-------------|---------------|-----------------------|-------------------------|
| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|-------------------------|-------------|---------------|-----------------------|-------------------------|

| | | | | |
|-----------------------------|------|------|-----------|-----|
| C8—H8...O9 ⁱ | 0.93 | 2.46 | 3.299 (4) | 150 |
| C9—H9...O7 ⁱ | 0.93 | 2.54 | 3.291 (4) | 138 |
| C38—H38...O11 ⁱⁱ | 0.93 | 2.58 | 3.457 (4) | 157 |
| C42—H42...O9 ⁱⁱⁱ | 0.93 | 2.42 | 3.259 (5) | 150 |
| C43—H43...O8 ⁱⁱⁱ | 0.93 | 2.57 | 3.316 (4) | 138 |

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

Fig. 1

