# Tris(dibenzoylmethanido-κ²O,O′)-[(6R,8R)-(−)-7,7-dimethyl-3-(2-pyridyl)-5,6,7,8-tetrahydro-6,8-methano-isoquinoline-κ²N,N′]terbium(III)

**Lei-Qi Chen,ᵃ Jian-Nan Guo,ᵇ Wei-Min Xuan,ᵃ Yi-Ji Linᵃ and Hui Zhangᵃ\***

ᵃDepartment of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, People's Republic of China, and ᵇThe Key Laboratory for Chemical Biology of Fujian Province, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, People's Republic of China

Correspondence e-mail: huizhang@xmu.edu.cn

In the title compound, $[Tb(C_{15}H_{11}O_2)_3(C_{17}H_{18}N_2)]$, the 7,7-dimethyl-3-(2-pyridyl)-5,6,7,8-tetrahydro-6,8-methanoisoquinoline ($L^{RR}$) ligand coordinates to Tb$^{III}$ through the two N atoms of the heterocycle. The metal centre is also chelated by three deprotonated 1,3-diphenylpropane-1,3-dione (dbm) ligands, forming enantiomerically pure $[Tb(dbm)_3L^{RR}]$. The Tb$^{III}$ atom is located in a distorted square antiprism of eight coordinating atoms (six O and two N atoms).

## Related literature

For a general background to lanthanide complexes, see: Aspinall (2002); Li, Chen et al. (2007); Li & Zhang (2008). For a related structure, see: Li, Zheng et al. (2007). For the synthesis, see: Hayoz et al. (1993); Lennartson et al. (2005).
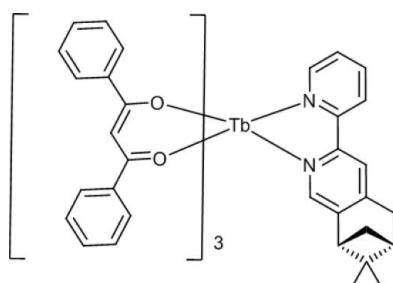


## Experimental

### Crystal data

$[Tb(C_{15}H_{11}O_2)_3(C_{17}H_{18}N_2)]$
$M_r = 1078.97$
Monoclinic, $P2_1$
$a = 9.5158$ (19) Å
$b = 20.790$ (4) Å
$c = 12.769$ (3) Å
$\beta = 92.47$ (3)°
$V = 2523.7$ (9) Å$^3$
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.46$ mm$^{-1}$
$T = 296$ K
$0.51 \times 0.43 \times 0.34$ mm

### Data collection

Rigaku R-AXIS SPIDER IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.524$, $T_{max} = 0.637$
19632 measured reflections
8346 independent reflections
5624 reflections with $I > 2\sigma(I)$
$R_{int} = 0.090$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.093$
$S = 0.95$
8346 reflections
640 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max} = 1.04$ e Å$^{-3}$
$\Delta\rho_{min} = -1.22$ e Å$^{-3}$
Absolute structure: Flack (1983), 3779 Friedel pairs
Flack parameter: −0.008 (14)

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

| | | | |
|---|---|---|---|
| N1—Tb1 | 2.589 (6) | Tb1—O4 | 2.353 (4) |
| Tb1—O2 | 2.328 (9) | Tb1—O6 | 2.372 (7) |
| Tb1—O3 | 2.312 (7) | Tb1—N2 | 2.569 (6) |
| Tb1—O5 | 2.341 (7) | | |

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2576).

## References

Aspinall, H. C. (2002). *Chem. Rev.* **102**, 1807–1850.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hayoz, P., Zelewsky, A. V. & Stoeckli-Evans, H. (1993). *J. Am. Chem. Soc.* **115**, 5111–5114.
Higashi, T. (1995). *ABSCOR.* Rigaku Corporation, Tokyo, Japan.
Lennartson, A., Vestergren, M. & Håkansson, M. (2005). *Chem. Eur. J.* **11**, 1757–1762.
Li, X. L., Chen, K., Liu, Y., Wang, Z. X., Wang, T. W., Zuo, J. L., Li, Y. Z., Wang, Y., Zhu, J. S., Liu, J. M., Song, Y. & You, X. Z. (2007). *Angew. Chem. Int. Ed.* **46**, 6820–6823.
Li, Z. F. & Zhang, H. J. (2008). *Chem. J. Chin. Univ.* **29**, 2597–2608.
Li, X. L., Zheng, Y. X., Zou, J. L., Song, Y. & You, X. Z. (2007). *Polyhedron*, **26**, 5257–5262.
Rigaku (1998). *PROCESS-AUTO.* Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure.* Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

## Tris(dibenzoylmethanido-*κ²O,O′*)[(6*R*,8*R*)-(−)-7,7-dimethyl-3-(2-pyridyl)-5,6,7,8-tetrahydro-6,8-methanoisoquinoline-*κ²N,N′*]terbium(III)

### Lei-Qi Chen, Jian-Nan Guo, Wei-Min Xuan, Yi-Ji Lin and Hui Zhang

### S1. Comment

Due to the potential applications as luminescence, ferroelectric material and NMR shift reagents, the stereoselective synthesis and characterization of labile lanthanide *β*-diketonate complexes have obtained a great deal of attentions (Aspinall, 2002; Li, Chen *et al.*, 2007); Li & Zhang, 2008). Herein, we report a chiral complex, [Tb(dbm)₃*LRR*] (Fig. 1), which is isostructural with the previously reported [Eu(dbm)₃*LRR*] (Li, Zheng *et al.*, 2007). For the intrducing of chiral ligand *LRR*, the complex was obtained as an enatiopure compound and crystallized in a chiral space group *P*2₁. The title compound, was synthesized under mild condition. *LRR* is introduced as a second ligand, which coordinates to Tbᴵᴵᴵ with three dbm to form enantiomerically pure complex [Tb(dbm)₃*LRR*]. The absolute configuration of the stereocenters in the ligand *LRR* remains unchanged during the synthetic procedure.

As indicated in Fig. 1, six O atoms and two N atoms come from the three diketone anions and a chiral 2,2-bipyridine derivative ligand, *LRR*, coordinate to a Tbᴵᴵᴵ cation to form a mononuclear neutral eight-coordinated Tbᴵᴵᴵ-based complex. In the distorted square antiprism around the Tbᴵᴵᴵ cation, O1, O2, N1, N2 and O3, O4, O5, O6 compose the top and bottom planes of the antiprism. The mean deviations from the two planes are 0.122 and 0.069 Å, and their dihedral angle is 1.83 (1)°. And the top plane is rotated by 37° relative to the bottom plane, which is smaller than 45° for a regular square antipism.

### S2. Experimental

The title compound was prepared *via* a modification of a previously reported method (Hayoz *et al.*, 1993; Lennartson *et al.*, 2005). The *LRR* ligand and [Tb(dbm)₃H₂O] was synthesized according to reported procedures.

A solution of [Tb(dbm)₃H₂O] (15 mg, 0.0178 mmol) in acetone (2 ml) was combined with a solution of (*8R,10R*)-(-)-[4,5]-pineno-2,2′-bipyridine (4.45 mg, 0.0178 mmol) in ethanol (2 ml). And the mixture was stand at room temperature for two days. Yellow block crystals of the title complex were obtained in 75% yield.

### S3. Refinement

The hydrogen atoms were positioned geometrically (C—H = 0.93, 0.98, 0.97 or 0.96Å for phenyl, tertiary, methylene or methyl H atoms respectively) and were included in the refinement in the riding model approximation. The displacement parameters of methyl H atoms were set to 1.5*U*ₑq(C), while those of other H atoms were set to 1.2*U*ₑq(C).
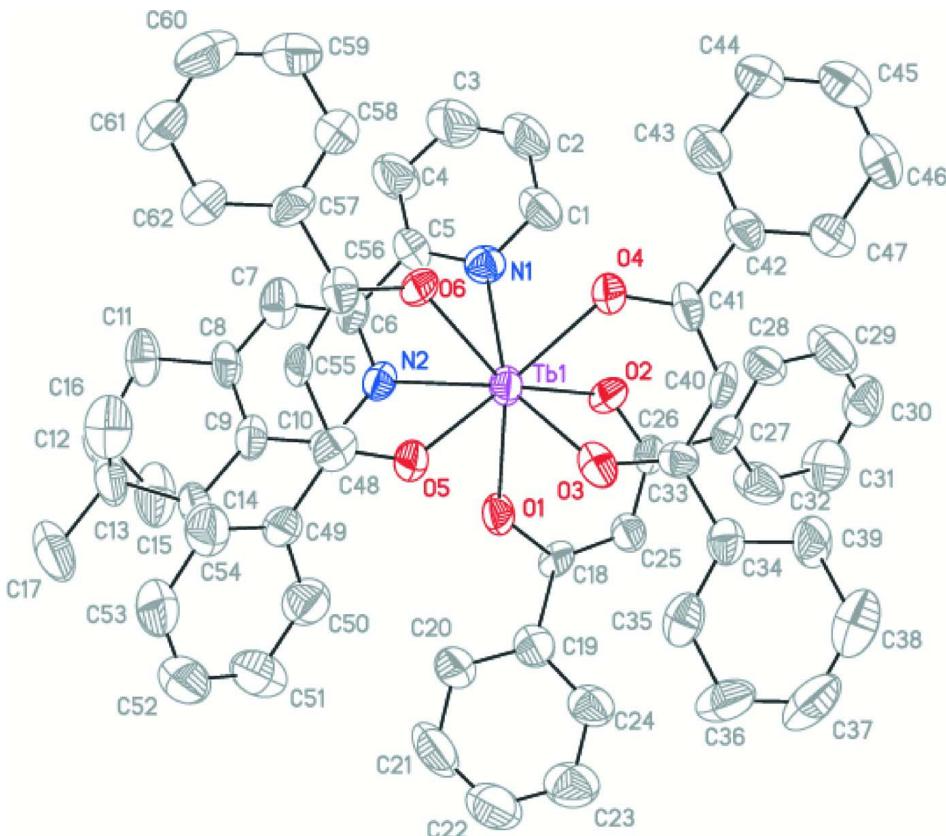
**Figure 1**

The structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids at the 50% probability level. The H atoms have been omited for charity.

**Tris(dibenzoylmethanido-$\kappa^2O,O'$)[(6$R$,8$R$)-(-)- 7,7-dimethyl-3-(2-pyridyl)-5,6,7,8-tetrahydro-6,8-methanoisoquinoline- $\kappa^2N,N'$]terbium(III)**

*Crystal data*
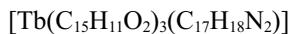
| | |
|---|---|
| [Tb(C$_{15}$H$_{11}$O$_2$)$_3$(C$_{17}$H$_{18}$N$_2$)] | $F(000) = 1100$ |
| $M_r = 1078.97$ | $D_x = 1.420$ Mg m$^{-3}$ |
| Monoclinic, $P2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2yb | Cell parameters from 11553 reflections |
| $a = 9.5158$ (19) Å | $\theta = 3.2–27.5°$ |
| $b = 20.790$ (4) Å | $\mu = 1.46$ mm$^{-1}$ |
| $c = 12.769$ (3) Å | $T = 296$ K |
| $\beta = 92.47$ (3)° | Block, yellow |
| $V = 2523.7$ (9) Å$^3$ | $0.51 \times 0.43 \times 0.34$ mm |
| $Z = 2$ | |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS SPIDER IP diffractometer | Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) |
| Radiation source: fine-focus sealed tube | $T_{min} = 0.524$, $T_{max} = 0.637$ |
| Graphite monochromator | 19632 measured reflections |
| $\omega$ scans | 8346 independent reflections |
| | 5624 reflections with $I > 2\sigma(I)$ |

$R_{int} = 0.090$

$\theta_{max} = 25.0°$, $\theta_{min} = 3.2°$

$h = -11 \rightarrow 11$

$k = -23 \rightarrow 24$

$l = -14 \rightarrow 15$

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.050$ | H-atom parameters constrained |
| $wR(F^2) = 0.093$ | $w = 1/[\sigma^2(F_o^2) + (0.0094P)^2 + 1.367P]$ |
| $S = 0.95$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 8346 reflections | $(\Delta/\sigma)_{max} = 0.003$ |
| 640 parameters | $\Delta\rho_{max} = 1.04$ e Å$^{-3}$ |
| 1 restraint | $\Delta\rho_{min} = -1.22$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 3779 Friedel pairs |
| Secondary atom site location: difference Fourier map | Absolute structure parameter: −0.008 (14) |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.3453 (11) | 0.4955 (5) | 1.0559 (7) | 0.061 (4) |
| H1A | 0.2627 | 0.4725 | 1.0640 | 0.073* |
| N1 | 0.3795 (6) | 0.5115 (7) | 0.9587 (4) | 0.0455 (15) |
| O1 | 0.2344 (7) | 0.4463 (3) | 0.6603 (6) | 0.044 (2) |
| Tb1 | 0.19194 (4) | 0.51094 (3) | 0.80567 (3) | 0.03880 (11) |
| C2 | 0.4251 (12) | 0.5109 (10) | 1.1437 (7) | 0.085 (3) |
| H2A | 0.3963 | 0.5000 | 1.2101 | 0.102* |
| N2 | 0.4480 (7) | 0.5358 (3) | 0.7640 (6) | 0.0378 (19) |
| O2 | 0.1996 (9) | 0.4047 (4) | 0.8634 (8) | 0.049 (3) |
| C3 | 0.5473 (15) | 0.5427 (6) | 1.1313 (10) | 0.099 (5) |
| H3A | 0.6048 | 0.5527 | 1.1897 | 0.118* |
| O3 | −0.0322 (7) | 0.4832 (2) | 0.7448 (5) | 0.0479 (17) |
| C4 | 0.5867 (12) | 0.5599 (5) | 1.0347 (9) | 0.076 (3) |
| H4A | 0.6697 | 0.5827 | 1.0266 | 0.091* |
| O4 | 0.0459 (5) | 0.5113 (5) | 0.9497 (3) | 0.0460 (13) |
| C5 | 0.5009 (11) | 0.5429 (4) | 0.9467 (7) | 0.049 (3) |
| O5 | 0.1579 (7) | 0.5793 (3) | 0.6611 (6) | 0.0403 (18) |
| C6 | 0.5388 (9) | 0.5584 (4) | 0.8388 (8) | 0.040 (2) |
| O6 | 0.2217 (10) | 0.6188 (3) | 0.8630 (8) | 0.047 (3) |
| C7 | 0.6570 (10) | 0.5914 (4) | 0.8162 (9) | 0.056 (3) |

| H7A | 0.7162 | 0.6067 | 0.8705 | 0.068* |
| C8 | 0.6903 (13) | 0.6027 (5) | 0.7130 (10) | 0.046 (3) |
| C9 | 0.6051 (10) | 0.5767 (4) | 0.6343 (8) | 0.047 (3) |
| C10 | 0.4818 (10) | 0.5450 (3) | 0.6637 (7) | 0.041 (2) |
| H10A | 0.4204 | 0.5295 | 0.6108 | 0.049* |
| C11 | 0.8151 (11) | 0.6428 (5) | 0.6816 (10) | 0.062 (3) |
| H11A | 0.9016 | 0.6237 | 0.7100 | 0.075* |
| H11B | 0.8077 | 0.6859 | 0.7100 | 0.075* |
| C12 | 0.8186 (12) | 0.6461 (5) | 0.5617 (10) | 0.060 (3) |
| H12A | 0.8977 | 0.6705 | 0.5352 | 0.072* |
| C13 | 0.6755 (16) | 0.6621 (6) | 0.5090 (11) | 0.065 (4) |
| C14 | 0.6401 (12) | 0.5886 (4) | 0.5235 (8) | 0.058 (3) |
| H14A | 0.5803 | 0.5681 | 0.4687 | 0.070* |
| C15 | 0.8052 (12) | 0.5770 (5) | 0.5200 (10) | 0.083 (4) |
| H15A | 0.8416 | 0.5443 | 0.5681 | 0.099* |
| H15B | 0.8392 | 0.5710 | 0.4501 | 0.099* |
| C16 | 0.5843 (11) | 0.7116 (5) | 0.5623 (9) | 0.069 (3) |
| H16A | 0.6169 | 0.7541 | 0.5467 | 0.104* |
| H16B | 0.5903 | 0.7049 | 0.6367 | 0.104* |
| H16C | 0.4884 | 0.7070 | 0.5370 | 0.104* |
| C17 | 0.6831 (14) | 0.6796 (6) | 0.3934 (9) | 0.104 (5) |
| H17A | 0.7039 | 0.7246 | 0.3870 | 0.155* |
| H17B | 0.5945 | 0.6705 | 0.3578 | 0.155* |
| H17C | 0.7558 | 0.6548 | 0.3626 | 0.155* |
| C18 | 0.1838 (15) | 0.3886 (6) | 0.6372 (12) | 0.047 (4) |
| C19 | 0.1776 (16) | 0.3760 (6) | 0.5217 (13) | 0.050 (4) |
| C20 | 0.2664 (15) | 0.4081 (6) | 0.4562 (11) | 0.067 (4) |
| H20A | 0.3296 | 0.4386 | 0.4832 | 0.080* |
| C21 | 0.260 (2) | 0.3937 (7) | 0.3468 (14) | 0.100 (7) |
| H21A | 0.3191 | 0.4149 | 0.3021 | 0.120* |
| C22 | 0.166 (2) | 0.3486 (9) | 0.3073 (14) | 0.094 (7) |
| H22A | 0.1597 | 0.3404 | 0.2357 | 0.113* |
| C23 | 0.0827 (14) | 0.3161 (5) | 0.3729 (10) | 0.076 (4) |
| H23A | 0.0206 | 0.2850 | 0.3463 | 0.091* |
| C24 | 0.0900 (13) | 0.3290 (4) | 0.4782 (8) | 0.059 (3) |
| H24A | 0.0340 | 0.3054 | 0.5221 | 0.070* |
| C25 | 0.1452 (11) | 0.3446 (4) | 0.7094 (7) | 0.043 (3) |
| H25A | 0.1067 | 0.3061 | 0.6846 | 0.052* |
| C26 | 0.1589 (10) | 0.3527 (4) | 0.8162 (7) | 0.037 (2) |
| C27 | 0.1249 (9) | 0.2964 (3) | 0.8876 (7) | 0.038 (2) |
| C28 | 0.0840 (12) | 0.3068 (4) | 0.9875 (7) | 0.062 (3) |
| H28A | 0.0795 | 0.3485 | 1.0133 | 0.074* |
| C29 | 0.0499 (13) | 0.2565 (5) | 1.0495 (8) | 0.085 (4) |
| H29A | 0.0217 | 0.2645 | 1.1171 | 0.102* |
| C30 | 0.0559 (12) | 0.1946 (4) | 1.0152 (9) | 0.067 (3) |
| H30A | 0.0297 | 0.1610 | 1.0583 | 0.080* |
| C31 | 0.1002 (13) | 0.1823 (5) | 0.9180 (10) | 0.079 (4) |
| H31A | 0.1089 | 0.1403 | 0.8944 | 0.095* |

| | | | | |
|------|------------------|-------------|--------------|-----------|
| C32 | 0.1324 (13) | 0.2336 (4) | 0.8546 (8) | 0.073 (4) |
| H32A | 0.1602 | 0.2254 | 0.7869 | 0.087* |
| C33 | −0.1299 (10) | 0.4515 (4) | 0.7860 (7) | 0.038 (2) |
| C34 | −0.2340 (12) | 0.4184 (5) | 0.7124 (9) | 0.043 (3) |
| C35 | −0.2038 (11) | 0.4120 (4) | 0.6077 (10) | 0.052 (3) |
| H35A | −0.1190 | 0.4277 | 0.5845 | 0.062* |
| C36 | −0.2997 (17) | 0.3822 (6) | 0.5360 (12) | 0.074 (5) |
| H36A | −0.2799 | 0.3795 | 0.4654 | 0.089* |
| C37 | −0.4207 (15) | 0.3576 (6) | 0.5704 (12) | 0.085 (4) |
| H37A | −0.4816 | 0.3355 | 0.5243 | 0.101* |
| C38 | −0.4543 (12) | 0.3653 (5) | 0.6740 (12) | 0.076 (4) |
| H38A | −0.5396 | 0.3496 | 0.6963 | 0.091* |
| C39 | −0.3618 (11) | 0.3964 (5) | 0.7463 (9) | 0.052 (3) |
| H39A | −0.3859 | 0.4022 | 0.8154 | 0.063* |
| C40 | −0.1415 (10) | 0.4455 (4) | 0.8923 (8) | 0.046 (2) |
| H40A | −0.2116 | 0.4184 | 0.9152 | 0.055* |
| C41 | −0.0589 (10) | 0.4760 (4) | 0.9682 (7) | 0.042 (2) |
| C42 | −0.0893 (10) | 0.4674 (4) | 1.0826 (7) | 0.048 (2) |
| C43 | −0.0303 (9) | 0.5112 (9) | 1.1547 (6) | 0.061 (2) |
| H43A | 0.0294 | 0.5434 | 1.1326 | 0.073* |
| C44 | −0.0616 (11) | 0.5064 (9) | 1.2606 (7) | 0.080 (3) |
| H44A | −0.0241 | 0.5360 | 1.3086 | 0.096* |
| C45 | −0.1463 (15) | 0.4586 (6) | 1.2936 (9) | 0.094 (4) |
| H45A | −0.1647 | 0.4553 | 1.3643 | 0.112* |
| C46 | −0.2038 (14) | 0.4162 (6) | 1.2253 (9) | 0.089 (4) |
| H46A | −0.2642 | 0.3848 | 1.2492 | 0.107* |
| C47 | −0.1749 (13) | 0.4182 (5) | 1.1191 (8) | 0.075 (4) |
| H47A | −0.2119 | 0.3872 | 1.0732 | 0.089* |
| C48 | 0.2014 (13) | 0.6338 (6) | 0.6362 (12) | 0.039 (4) |
| C49 | 0.1978 (14) | 0.6503 (6) | 0.5226 (13) | 0.041 (4) |
| C50 | 0.2037 (14) | 0.5989 (6) | 0.4524 (12) | 0.061 (4) |
| H50A | 0.2033 | 0.5570 | 0.4777 | 0.073* |
| C51 | 0.2099 (19) | 0.6093 (8) | 0.3490 (14) | 0.085 (5) |
| H51A | 0.2173 | 0.5745 | 0.3037 | 0.103* |
| C52 | 0.2054 (16) | 0.6708 (10) | 0.3091 (14) | 0.081 (6) |
| H52A | 0.2059 | 0.6774 | 0.2371 | 0.097* |
| C53 | 0.2004 (14) | 0.7212 (5) | 0.3744 (10) | 0.073 (4) |
| H53A | 0.1987 | 0.7628 | 0.3477 | 0.088* |
| C54 | 0.1977 (12) | 0.7112 (5) | 0.4813 (9) | 0.061 (3) |
| H54A | 0.1957 | 0.7464 | 0.5261 | 0.073* |
| C55 | 0.2517 (10) | 0.6806 (4) | 0.7104 (7) | 0.039 (2) |
| H55A | 0.2743 | 0.7212 | 0.6857 | 0.047* |
| C56 | 0.2688 (11) | 0.6690 (4) | 0.8176 (8) | 0.041 (2) |
| C57 | 0.3457 (10) | 0.7162 (4) | 0.8887 (8) | 0.049 (3) |
| C58 | 0.3327 (13) | 0.7120 (5) | 0.9947 (9) | 0.077 (4) |
| H58A | 0.2728 | 0.6816 | 1.0221 | 0.092* |
| C59 | 0.4101 (18) | 0.7536 (8) | 1.0620 (12) | 0.106 (5) |
| H59A | 0.4028 | 0.7504 | 1.1343 | 0.127* |

| | | | |
|---|---|---|---|
| C60 | 0.4949 (13) | 0.7981 (6) | 1.0211 (12) | 0.082 (4) |
| H60A | 0.5484 | 0.8248 | 1.0657 | 0.098* |
| C61 | 0.5031 (16) | 0.8045 (6) | 0.9181 (12) | 0.089 (5) |
| H61A | 0.5586 | 0.8369 | 0.8913 | 0.106* |
| C62 | 0.4301 (12) | 0.7636 (4) | 0.8507 (9) | 0.072 (3) |
| H62B | 0.4381 | 0.7680 | 0.7787 | 0.087* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.073 (8) | 0.068 (10) | 0.041 (6) | −0.002 (5) | 0.011 (5) | 0.009 (5) |
| N1 | 0.046 (4) | 0.046 (3) | 0.045 (4) | 0.001 (8) | 0.006 (3) | −0.008 (9) |
| O1 | 0.039 (5) | 0.045 (4) | 0.049 (4) | −0.009 (3) | 0.016 (4) | 0.001 (3) |
| Tb1 | 0.0427 (2) | 0.03169 (16) | 0.0427 (2) | −0.0053 (4) | 0.01018 (15) | 0.0003 (4) |
| C2 | 0.100 (9) | 0.116 (8) | 0.039 (6) | −0.024 (15) | 0.003 (6) | 0.013 (15) |
| N2 | 0.028 (5) | 0.037 (4) | 0.050 (5) | −0.007 (3) | 0.010 (4) | −0.007 (3) |
| O2 | 0.051 (6) | 0.047 (5) | 0.049 (7) | −0.014 (4) | 0.002 (5) | −0.013 (4) |
| C3 | 0.097 (12) | 0.143 (12) | 0.054 (9) | −0.036 (9) | −0.010 (8) | 0.006 (7) |
| O3 | 0.054 (5) | 0.049 (3) | 0.042 (4) | −0.001 (3) | 0.014 (3) | 0.007 (3) |
| C4 | 0.058 (9) | 0.122 (9) | 0.048 (8) | −0.019 (7) | −0.001 (6) | 0.007 (7) |
| O4 | 0.046 (3) | 0.050 (3) | 0.043 (3) | −0.015 (6) | 0.014 (3) | −0.004 (7) |
| C5 | 0.050 (7) | 0.057 (5) | 0.042 (6) | −0.001 (5) | 0.012 (5) | 0.008 (4) |
| O5 | 0.045 (5) | 0.034 (3) | 0.042 (4) | −0.009 (3) | 0.002 (4) | 0.002 (3) |
| C6 | 0.026 (6) | 0.035 (4) | 0.060 (7) | −0.004 (4) | 0.006 (5) | 0.003 (4) |
| O6 | 0.072 (7) | 0.024 (4) | 0.047 (7) | −0.011 (4) | 0.014 (5) | −0.015 (4) |
| C7 | 0.037 (7) | 0.062 (6) | 0.069 (8) | −0.007 (5) | −0.014 (6) | 0.021 (6) |
| C8 | 0.031 (8) | 0.053 (6) | 0.055 (8) | −0.010 (6) | 0.022 (7) | 0.008 (5) |
| C9 | 0.048 (7) | 0.033 (5) | 0.063 (7) | −0.005 (4) | 0.022 (6) | −0.006 (4) |
| C10 | 0.048 (7) | 0.042 (4) | 0.034 (6) | −0.006 (4) | 0.007 (5) | −0.014 (4) |
| C11 | 0.033 (6) | 0.062 (6) | 0.091 (10) | −0.004 (5) | 0.004 (6) | 0.031 (7) |
| C12 | 0.041 (8) | 0.052 (7) | 0.089 (10) | 0.000 (5) | 0.026 (7) | 0.007 (6) |
| C13 | 0.078 (10) | 0.048 (7) | 0.070 (10) | −0.013 (6) | 0.035 (8) | 0.010 (6) |
| C14 | 0.076 (9) | 0.054 (6) | 0.047 (7) | −0.022 (5) | 0.023 (6) | −0.001 (5) |
| C15 | 0.076 (10) | 0.058 (7) | 0.117 (11) | 0.005 (6) | 0.050 (9) | 0.003 (7) |
| C16 | 0.047 (7) | 0.059 (6) | 0.102 (10) | 0.012 (5) | 0.002 (7) | 0.024 (7) |
| C17 | 0.117 (12) | 0.122 (10) | 0.073 (10) | −0.041 (9) | 0.015 (9) | 0.038 (8) |
| C18 | 0.067 (11) | 0.020 (7) | 0.055 (10) | −0.011 (5) | 0.015 (8) | −0.023 (6) |
| C19 | 0.067 (11) | 0.037 (8) | 0.048 (10) | 0.004 (6) | 0.014 (8) | −0.006 (7) |
| C20 | 0.096 (12) | 0.057 (7) | 0.047 (8) | −0.020 (7) | 0.003 (8) | 0.007 (6) |
| C21 | 0.18 (2) | 0.076 (11) | 0.052 (11) | −0.023 (11) | 0.040 (11) | 0.014 (8) |
| C22 | 0.156 (18) | 0.075 (12) | 0.052 (13) | −0.010 (10) | 0.002 (12) | 0.007 (8) |
| C23 | 0.094 (12) | 0.070 (8) | 0.063 (9) | 0.004 (7) | 0.004 (8) | −0.016 (6) |
| C24 | 0.086 (10) | 0.044 (6) | 0.047 (7) | 0.000 (6) | 0.012 (7) | −0.006 (5) |
| C25 | 0.060 (8) | 0.033 (5) | 0.039 (6) | −0.004 (5) | 0.015 (6) | −0.004 (4) |
| C26 | 0.036 (7) | 0.028 (4) | 0.048 (6) | −0.005 (4) | 0.001 (5) | 0.007 (4) |
| C27 | 0.040 (6) | 0.026 (4) | 0.049 (6) | −0.005 (4) | 0.003 (5) | −0.002 (4) |
| C28 | 0.092 (10) | 0.053 (6) | 0.041 (7) | −0.013 (6) | 0.011 (6) | 0.003 (5) |
| C29 | 0.119 (13) | 0.081 (8) | 0.057 (8) | −0.003 (7) | 0.034 (8) | 0.006 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C30 | 0.075 (9) | 0.048 (6) | 0.077 (9) | −0.014 (5) | −0.009 (7) | 0.023 (6) |
| C31 | 0.111 (11) | 0.044 (6) | 0.082 (9) | −0.006 (6) | 0.003 (8) | 0.013 (6) |
| C32 | 0.118 (11) | 0.049 (6) | 0.052 (7) | 0.004 (6) | 0.017 (7) | −0.003 (5) |
| C33 | 0.046 (7) | 0.040 (5) | 0.029 (5) | 0.004 (4) | −0.001 (5) | 0.000 (4) |
| C34 | 0.041 (8) | 0.037 (5) | 0.052 (7) | −0.003 (5) | 0.007 (6) | 0.003 (4) |
| C35 | 0.048 (7) | 0.032 (5) | 0.074 (9) | 0.000 (4) | −0.005 (6) | 0.010 (6) |
| C36 | 0.092 (13) | 0.064 (10) | 0.063 (10) | −0.011 (8) | −0.021 (8) | −0.016 (7) |
| C37 | 0.071 (11) | 0.071 (8) | 0.108 (13) | −0.023 (7) | −0.043 (9) | −0.003 (8) |
| C38 | 0.043 (8) | 0.063 (7) | 0.120 (12) | −0.008 (5) | −0.005 (8) | 0.008 (7) |
| C39 | 0.028 (7) | 0.075 (7) | 0.054 (8) | −0.007 (5) | 0.001 (6) | 0.012 (6) |
| C40 | 0.034 (6) | 0.046 (5) | 0.057 (7) | −0.021 (4) | 0.004 (5) | 0.003 (4) |
| C41 | 0.034 (6) | 0.042 (5) | 0.052 (6) | 0.000 (4) | 0.024 (5) | 0.008 (4) |
| C42 | 0.042 (7) | 0.057 (5) | 0.044 (6) | 0.002 (4) | 0.012 (5) | −0.001 (5) |
| C43 | 0.077 (6) | 0.057 (4) | 0.049 (5) | 0.002 (12) | 0.016 (5) | 0.009 (12) |
| C44 | 0.114 (9) | 0.082 (7) | 0.046 (6) | −0.029 (12) | 0.018 (6) | −0.010 (10) |
| C45 | 0.127 (13) | 0.113 (10) | 0.042 (8) | −0.036 (9) | 0.020 (8) | −0.005 (7) |
| C46 | 0.114 (12) | 0.103 (9) | 0.052 (8) | −0.041 (8) | 0.026 (8) | 0.014 (6) |
| C47 | 0.100 (10) | 0.075 (7) | 0.051 (7) | −0.028 (6) | 0.025 (7) | −0.014 (5) |
| C48 | 0.015 (7) | 0.046 (8) | 0.054 (10) | 0.005 (5) | 0.000 (6) | −0.008 (7) |
| C49 | 0.033 (8) | 0.046 (8) | 0.043 (10) | −0.005 (6) | −0.002 (7) | −0.004 (7) |
| C50 | 0.067 (10) | 0.055 (7) | 0.060 (9) | −0.002 (6) | −0.008 (7) | 0.003 (6) |
| C51 | 0.123 (14) | 0.083 (10) | 0.051 (10) | −0.009 (9) | 0.005 (9) | 0.003 (7) |
| C52 | 0.083 (13) | 0.114 (17) | 0.047 (12) | −0.029 (10) | 0.007 (9) | 0.004 (10) |
| C53 | 0.096 (11) | 0.062 (7) | 0.063 (9) | −0.019 (7) | −0.002 (8) | 0.023 (6) |
| C54 | 0.071 (9) | 0.049 (6) | 0.064 (8) | −0.007 (6) | 0.010 (7) | 0.004 (5) |
| C55 | 0.049 (7) | 0.025 (4) | 0.043 (6) | −0.009 (4) | 0.008 (5) | 0.006 (4) |
| C56 | 0.041 (7) | 0.029 (5) | 0.055 (7) | 0.002 (4) | 0.012 (5) | 0.006 (4) |
| C57 | 0.055 (7) | 0.037 (5) | 0.055 (7) | −0.001 (4) | 0.005 (5) | −0.015 (4) |
| C58 | 0.104 (11) | 0.070 (7) | 0.057 (8) | −0.039 (7) | 0.010 (7) | −0.006 (6) |
| C59 | 0.130 (16) | 0.131 (14) | 0.056 (9) | −0.052 (11) | 0.006 (10) | −0.028 (9) |
| C60 | 0.067 (10) | 0.089 (9) | 0.090 (11) | −0.009 (7) | −0.008 (8) | −0.039 (8) |
| C61 | 0.104 (13) | 0.078 (9) | 0.085 (12) | −0.046 (8) | 0.016 (10) | −0.027 (8) |
| C62 | 0.093 (10) | 0.063 (6) | 0.061 (8) | −0.033 (6) | 0.007 (7) | −0.013 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.338 (10) | C25—H25A | 0.9300 |
| C1—C2 | 1.365 (13) | C26—C27 | 1.525 (10) |
| C1—H1A | 0.9300 | C27—C28 | 1.367 (11) |
| N1—C5 | 1.342 (12) | C27—C32 | 1.375 (11) |
| N1—Tb1 | 2.589 (6) | C28—C29 | 1.360 (12) |
| O1—C18 | 1.321 (13) | C28—H28A | 0.9300 |
| O1—Tb1 | 2.341 (7) | C29—C30 | 1.360 (13) |
| Tb1—O2 | 2.328 (9) | C29—H29A | 0.9300 |
| Tb1—O3 | 2.312 (7) | C30—C31 | 1.352 (14) |
| Tb1—O5 | 2.341 (7) | C30—H30A | 0.9300 |
| Tb1—O4 | 2.353 (4) | C31—C32 | 1.382 (12) |
| Tb1—O6 | 2.372 (7) | C31—H31A | 0.9300 |

| | | | |
|---|---|---|---|
| Tb1—N2 | 2.569 (6) | C32—H32A | 0.9300 |
| C2—C3 | 1.352 (16) | C33—C40 | 1.372 (11) |
| C2—H2A | 0.9300 | C33—C34 | 1.503 (14) |
| N2—C6 | 1.344 (11) | C34—C35 | 1.385 (16) |
| N2—C10 | 1.348 (10) | C34—C39 | 1.386 (13) |
| O2—C26 | 1.290 (11) | C35—C36 | 1.409 (16) |
| C3—C4 | 1.353 (14) | C35—H35A | 0.9300 |
| C3—H3A | 0.9300 | C36—C37 | 1.350 (18) |
| O3—C33 | 1.272 (9) | C36—H36A | 0.9300 |
| C4—C5 | 1.405 (14) | C37—C38 | 1.384 (16) |
| C4—H4A | 0.9300 | C37—H37A | 0.9300 |
| O4—C41 | 1.267 (10) | C38—C39 | 1.405 (15) |
| C5—C6 | 1.475 (12) | C38—H38A | 0.9300 |
| O5—C48 | 1.253 (14) | C39—H39A | 0.9300 |
| C6—C7 | 1.360 (11) | C40—C41 | 1.376 (12) |
| O6—C56 | 1.284 (11) | C40—H40A | 0.9300 |
| C7—C8 | 1.388 (15) | C41—C42 | 1.513 (12) |
| C7—H7A | 0.9300 | C42—C43 | 1.395 (16) |
| C8—C9 | 1.374 (15) | C42—C47 | 1.401 (12) |
| C8—C11 | 1.519 (13) | C43—C44 | 1.400 (10) |
| C9—C10 | 1.411 (11) | C43—H43A | 0.9300 |
| C9—C14 | 1.489 (12) | C44—C45 | 1.357 (18) |
| C10—H10A | 0.9300 | C44—H44A | 0.9300 |
| C11—C12 | 1.533 (16) | C45—C46 | 1.340 (15) |
| C11—H11A | 0.9700 | C45—H45A | 0.9300 |
| C11—H11B | 0.9700 | C46—C47 | 1.396 (13) |
| C12—C13 | 1.530 (18) | C46—H46A | 0.9300 |
| C12—C15 | 1.535 (13) | C47—H47A | 0.9300 |
| C12—H12A | 0.9800 | C48—C55 | 1.425 (16) |
| C13—C16 | 1.524 (16) | C48—C49 | 1.49 (2) |
| C13—C17 | 1.526 (16) | C49—C54 | 1.372 (16) |
| C13—C14 | 1.577 (13) | C49—C50 | 1.397 (18) |
| C14—C15 | 1.592 (15) | C50—C51 | 1.34 (2) |
| C14—H14A | 0.9800 | C50—H50A | 0.9300 |
| C15—H15A | 0.9700 | C51—C52 | 1.38 (2) |
| C15—H15B | 0.9700 | C51—H51A | 0.9300 |
| C16—H16A | 0.9600 | C52—C53 | 1.34 (2) |
| C16—H16B | 0.9600 | C52—H52A | 0.9300 |
| C16—H16C | 0.9600 | C53—C54 | 1.382 (14) |
| C17—H17A | 0.9600 | C53—H53A | 0.9300 |
| C17—H17B | 0.9600 | C54—H54A | 0.9300 |
| C17—H17C | 0.9600 | C55—C56 | 1.393 (12) |
| C18—C25 | 1.361 (16) | C55—H55A | 0.9300 |
| C18—C19 | 1.50 (2) | C56—C57 | 1.506 (12) |
| C19—C24 | 1.385 (17) | C57—C58 | 1.367 (13) |
| C19—C20 | 1.385 (17) | C57—C62 | 1.372 (12) |
| C20—C21 | 1.43 (2) | C58—C59 | 1.406 (16) |
| C20—H20A | 0.9300 | C58—H58A | 0.9300 |

| | | | |
|---|---|---|---|
| C21—C22 | 1.38 (2) | C59—C60 | 1.348 (17) |
| C21—H21A | 0.9300 | C59—H59A | 0.9300 |
| C22—C23 | 1.358 (19) | C60—C61 | 1.328 (17) |
| C22—H22A | 0.9300 | C60—H60A | 0.9300 |
| C23—C24 | 1.370 (14) | C61—C62 | 1.377 (15) |
| C23—H23A | 0.9300 | C61—H61A | 0.9300 |
| C24—H24A | 0.9300 | C62—H62B | 0.9300 |
| C25—C26 | 1.374 (12) | | |
| | | | |
| N1—C1—C2 | 123.6 (10) | C23—C22—C21 | 120.0 (17) |
| N1—C1—H1A | 118.2 | C23—C22—H22A | 120.0 |
| C2—C1—H1A | 118.2 | C21—C22—H22A | 120.0 |
| C5—N1—C1 | 118.2 (8) | C22—C23—C24 | 120.1 (14) |
| C5—N1—Tb1 | 119.0 (7) | C22—C23—H23A | 120.0 |
| C1—N1—Tb1 | 120.8 (6) | C24—C23—H23A | 120.0 |
| C18—O1—Tb1 | 128.7 (7) | C19—C24—C23 | 122.4 (12) |
| O2—Tb1—O3 | 83.4 (3) | C19—C24—H24A | 118.8 |
| O2—Tb1—O5 | 145.8 (3) | C23—C24—H24A | 118.8 |
| O3—Tb1—O5 | 78.0 (2) | C18—C25—C26 | 125.0 (9) |
| O2—Tb1—O1 | 72.7 (3) | C18—C25—H25A | 117.5 |
| O3—Tb1—O1 | 77.2 (2) | C26—C25—H25A | 117.5 |
| O5—Tb1—O1 | 75.32 (17) | O2—C26—C25 | 125.4 (8) |
| O2—Tb1—O4 | 76.5 (3) | O2—C26—C27 | 115.5 (9) |
| O3—Tb1—O4 | 72.31 (19) | C25—C26—C27 | 119.0 (8) |
| O5—Tb1—O4 | 123.3 (3) | C28—C27—C32 | 117.1 (8) |
| O1—Tb1—O4 | 138.5 (3) | C28—C27—C26 | 120.9 (7) |
| O2—Tb1—O6 | 142.88 (17) | C32—C27—C26 | 122.0 (8) |
| O3—Tb1—O6 | 115.8 (3) | C27—C28—C29 | 120.5 (9) |
| O5—Tb1—O6 | 71.3 (3) | C27—C28—H28A | 119.8 |
| O1—Tb1—O6 | 139.9 (3) | C29—C28—H28A | 119.8 |
| O4—Tb1—O6 | 79.8 (3) | C30—C29—C28 | 121.7 (10) |
| O2—Tb1—N2 | 103.9 (3) | C30—C29—H29A | 119.1 |
| O3—Tb1—N2 | 148.2 (2) | C28—C29—H29A | 119.1 |
| O5—Tb1—N2 | 79.3 (2) | C29—C30—C31 | 119.5 (9) |
| O1—Tb1—N2 | 75.7 (2) | C29—C30—H30A | 120.2 |
| O4—Tb1—N2 | 139.4 (2) | C31—C30—H30A | 120.2 |
| O6—Tb1—N2 | 76.8 (2) | C30—C31—C32 | 118.6 (10) |
| O2—Tb1—N1 | 75.8 (4) | C30—C31—H31A | 120.7 |
| O3—Tb1—N1 | 148.3 (2) | C32—C31—H31A | 120.7 |
| O5—Tb1—N1 | 131.3 (3) | C27—C32—C31 | 122.5 (10) |
| O1—Tb1—N1 | 117.7 (3) | C27—C32—H32A | 118.7 |
| O4—Tb1—N1 | 79.69 (17) | C31—C32—H32A | 118.7 |
| O6—Tb1—N1 | 72.2 (4) | O3—C33—C40 | 123.2 (9) |
| N2—Tb1—N1 | 61.7 (2) | O3—C33—C34 | 116.8 (8) |
| C3—C2—C1 | 118.0 (10) | C40—C33—C34 | 120.0 (8) |
| C3—C2—H2A | 121.0 | C35—C34—C39 | 119.4 (11) |
| C1—C2—H2A | 121.0 | C35—C34—C33 | 119.3 (9) |
| C6—N2—C10 | 117.0 (7) | C39—C34—C33 | 121.2 (10) |

| | | | |
|---|---|---|---|
| C6—N2—Tb1 | 120.7 (5) | C34—C35—C36 | 120.9 (11) |
| C10—N2—Tb1 | 119.5 (6) | C34—C35—H35A | 119.5 |
| C26—O2—Tb1 | 130.0 (8) | C36—C35—H35A | 119.5 |
| C2—C3—C4 | 120.7 (12) | C37—C36—C35 | 119.6 (14) |
| C2—C3—H3A | 119.7 | C37—C36—H36A | 120.2 |
| C4—C3—H3A | 119.7 | C35—C36—H36A | 120.2 |
| C33—O3—Tb1 | 132.1 (6) | C36—C37—C38 | 120.2 (12) |
| C3—C4—C5 | 119.2 (11) | C36—C37—H37A | 119.9 |
| C3—C4—H4A | 120.4 | C38—C37—H37A | 119.9 |
| C5—C4—H4A | 120.4 | C37—C38—C39 | 121.1 (11) |
| C41—O4—Tb1 | 129.8 (6) | C37—C38—H38A | 119.4 |
| N1—C5—C4 | 120.3 (8) | C39—C38—H38A | 119.4 |
| N1—C5—C6 | 117.3 (9) | C34—C39—C38 | 118.7 (11) |
| C4—C5—C6 | 122.4 (9) | C34—C39—H39A | 120.6 |
| C48—O5—Tb1 | 135.5 (8) | C38—C39—H39A | 120.6 |
| N2—C6—C7 | 122.6 (9) | C33—C40—C41 | 126.0 (8) |
| N2—C6—C5 | 114.3 (8) | C33—C40—H40A | 117.0 |
| C7—C6—C5 | 123.1 (10) | C41—C40—H40A | 117.0 |
| C56—O6—Tb1 | 132.0 (7) | O4—C41—C40 | 124.5 (8) |
| C6—C7—C8 | 120.8 (11) | O4—C41—C42 | 115.7 (9) |
| C6—C7—H7A | 119.6 | C40—C41—C42 | 119.9 (8) |
| C8—C7—H7A | 119.6 | C43—C42—C47 | 118.7 (9) |
| C9—C8—C7 | 118.4 (9) | C43—C42—C41 | 118.1 (8) |
| C9—C8—C11 | 117.8 (10) | C47—C42—C41 | 123.1 (9) |
| C7—C8—C11 | 123.8 (12) | C42—C43—C44 | 119.6 (14) |
| C8—C9—C10 | 117.5 (9) | C42—C43—H43A | 120.2 |
| C8—C9—C14 | 118.7 (9) | C44—C43—H43A | 120.2 |
| C10—C9—C14 | 123.6 (10) | C45—C44—C43 | 120.4 (15) |
| N2—C10—C9 | 123.6 (9) | C45—C44—H44A | 119.8 |
| N2—C10—H10A | 118.2 | C43—C44—H44A | 119.8 |
| C9—C10—H10A | 118.2 | C46—C45—C44 | 120.7 (11) |
| C8—C11—C12 | 109.8 (10) | C46—C45—H45A | 119.6 |
| C8—C11—H11A | 109.7 | C44—C45—H45A | 119.6 |
| C12—C11—H11A | 109.7 | C45—C46—C47 | 121.4 (11) |
| C8—C11—H11B | 109.7 | C45—C46—H46A | 119.3 |
| C12—C11—H11B | 109.7 | C47—C46—H46A | 119.3 |
| H11A—C11—H11B | 108.2 | C46—C47—C42 | 119.1 (10) |
| C13—C12—C11 | 113.1 (9) | C46—C47—H47A | 120.4 |
| C13—C12—C15 | 89.5 (10) | C42—C47—H47A | 120.4 |
| C11—C12—C15 | 107.4 (9) | O5—C48—C55 | 123.6 (13) |
| C13—C12—H12A | 114.7 | O5—C48—C49 | 117.4 (12) |
| C11—C12—H12A | 114.7 | C55—C48—C49 | 119.0 (12) |
| C15—C12—H12A | 114.7 | C54—C49—C50 | 117.3 (14) |
| C16—C13—C17 | 108.8 (10) | C54—C49—C48 | 125.8 (13) |
| C16—C13—C12 | 117.6 (12) | C50—C49—C48 | 116.8 (13) |
| C17—C13—C12 | 113.5 (10) | C51—C50—C49 | 120.9 (14) |
| C16—C13—C14 | 118.2 (9) | C51—C50—H50A | 119.6 |
| C17—C13—C14 | 111.3 (11) | C49—C50—H50A | 119.6 |

| | | | |
|---|---|---|---|
| C12—C13—C14 | 85.9 (9) | C50—C51—C52 | 120.7 (16) |
| C9—C14—C13 | 109.3 (8) | C50—C51—H51A | 119.6 |
| C9—C14—C15 | 105.3 (9) | C52—C51—H51A | 119.6 |
| C13—C14—C15 | 85.9 (8) | C53—C52—C51 | 119.8 (16) |
| C9—C14—H14A | 117.3 | C53—C52—H52A | 120.1 |
| C13—C14—H14A | 117.3 | C51—C52—H52A | 120.1 |
| C15—C14—H14A | 117.3 | C52—C53—C54 | 120.0 (12) |
| C12—C15—C14 | 85.2 (7) | C52—C53—H53A | 120.0 |
| C12—C15—H15A | 114.5 | C54—C53—H53A | 120.0 |
| C14—C15—H15A | 114.5 | C49—C54—C53 | 121.2 (11) |
| C12—C15—H15B | 114.5 | C49—C54—H54A | 119.4 |
| C14—C15—H15B | 114.5 | C53—C54—H54A | 119.4 |
| H15A—C15—H15B | 111.6 | C56—C55—C48 | 123.8 (9) |
| C13—C16—H16A | 109.5 | C56—C55—H55A | 118.1 |
| C13—C16—H16B | 109.5 | C48—C55—H55A | 118.1 |
| H16A—C16—H16B | 109.5 | O6—C56—C55 | 123.8 (9) |
| C13—C16—H16C | 109.5 | O6—C56—C57 | 115.4 (9) |
| H16A—C16—H16C | 109.5 | C55—C56—C57 | 120.9 (8) |
| H16B—C16—H16C | 109.5 | C58—C57—C62 | 118.4 (9) |
| C13—C17—H17A | 109.5 | C58—C57—C56 | 119.5 (9) |
| C13—C17—H17B | 109.5 | C62—C57—C56 | 122.1 (9) |
| H17A—C17—H17B | 109.5 | C57—C58—C59 | 119.9 (11) |
| C13—C17—H17C | 109.5 | C57—C58—H58A | 120.1 |
| H17A—C17—H17C | 109.5 | C59—C58—H58A | 120.1 |
| H17B—C17—H17C | 109.5 | C60—C59—C58 | 119.5 (13) |
| O1—C18—C25 | 124.4 (12) | C60—C59—H59A | 120.3 |
| O1—C18—C19 | 112.2 (12) | C58—C59—H59A | 120.3 |
| C25—C18—C19 | 123.4 (11) | C61—C60—C59 | 120.9 (13) |
| C24—C19—C20 | 118.0 (14) | C61—C60—H60A | 119.5 |
| C24—C19—C18 | 121.0 (13) | C59—C60—H60A | 119.5 |
| C20—C19—C18 | 120.8 (14) | C60—C61—C62 | 120.5 (12) |
| C19—C20—C21 | 119.2 (14) | C60—C61—H61A | 119.7 |
| C19—C20—H20A | 120.4 | C62—C61—H61A | 119.7 |
| C21—C20—H20A | 120.4 | C61—C62—C57 | 120.6 (11) |
| C22—C21—C20 | 120.1 (15) | C61—C62—H62B | 119.7 |
| C22—C21—H21A | 119.9 | C57—C62—H62B | 119.7 |
| C20—C21—H21A | 119.9 | | |
| | | | |
| C2—C1—N1—C5 | 2 (2) | C8—C9—C14—C13 | −45.9 (14) |
| C2—C1—N1—Tb1 | −161.5 (13) | C10—C9—C14—C13 | 128.2 (10) |
| C18—O1—Tb1—O2 | 36.6 (11) | C8—C9—C14—C15 | 45.0 (12) |
| C18—O1—Tb1—O3 | −50.4 (11) | C10—C9—C14—C15 | −140.9 (9) |
| C18—O1—Tb1—O5 | −131.1 (11) | C16—C13—C14—C9 | −41.5 (16) |
| C18—O1—Tb1—O4 | −7.1 (12) | C17—C13—C14—C9 | −168.5 (11) |
| C18—O1—Tb1—O6 | −165.4 (10) | C12—C13—C14—C9 | 77.8 (10) |
| C18—O1—Tb1—N2 | 146.4 (11) | C16—C13—C14—C15 | −146.2 (13) |
| C18—O1—Tb1—N1 | 99.7 (11) | C17—C13—C14—C15 | 86.7 (11) |
| C5—N1—Tb1—O2 | 135.2 (9) | C12—C13—C14—C15 | −26.9 (8) |

| | | | |
|---|---|---|---|
| C1—N1—Tb1—O2 | −61.4 (10) | C13—C12—C15—C14 | −27.7 (8) |
| C5—N1—Tb1—O3 | −174.3 (6) | C11—C12—C15—C14 | 86.4 (9) |
| C1—N1—Tb1—O3 | −10.8 (14) | C9—C14—C15—C12 | −82.0 (8) |
| C5—N1—Tb1—O5 | −20.7 (10) | C13—C14—C15—C12 | 26.9 (9) |
| C1—N1—Tb1—O5 | 142.8 (9) | Tb1—O1—C18—C25 | −28.7 (19) |
| C5—N1—Tb1—O1 | 73.9 (10) | Tb1—O1—C18—C19 | 153.1 (9) |
| C1—N1—Tb1—O1 | −122.7 (9) | O1—C18—C19—C24 | −159.4 (12) |
| C5—N1—Tb1—O4 | −146.3 (9) | C25—C18—C19—C24 | 22 (2) |
| C1—N1—Tb1—O4 | 17.2 (10) | O1—C18—C19—C20 | 25 (2) |
| C5—N1—Tb1—O6 | −63.8 (9) | C25—C18—C19—C20 | −153.2 (13) |
| C1—N1—Tb1—O6 | 99.7 (10) | C24—C19—C20—C21 | 3 (2) |
| C5—N1—Tb1—N2 | 20.6 (7) | C18—C19—C20—C21 | 178.5 (15) |
| C1—N1—Tb1—N2 | −176.0 (12) | C19—C20—C21—C22 | 0 (3) |
| N1—C1—C2—C3 | −2 (3) | C20—C21—C22—C23 | −2 (3) |
| O2—Tb1—N2—C6 | −88.2 (6) | C21—C22—C23—C24 | 1 (3) |
| O3—Tb1—N2—C6 | 171.8 (5) | C20—C19—C24—C23 | −4 (2) |
| O5—Tb1—N2—C6 | 126.7 (6) | C18—C19—C24—C23 | −179.5 (13) |
| O1—Tb1—N2—C6 | −155.9 (6) | C22—C23—C24—C19 | 2 (2) |
| O4—Tb1—N2—C6 | −2.9 (8) | O1—C18—C25—C26 | −3 (2) |
| O6—Tb1—N2—C6 | 53.6 (6) | C19—C18—C25—C26 | 175.1 (13) |
| N1—Tb1—N2—C6 | −23.0 (6) | Tb1—O2—C26—C25 | 23.7 (16) |
| O2—Tb1—N2—C10 | 111.7 (5) | Tb1—O2—C26—C27 | −156.6 (6) |
| O3—Tb1—N2—C10 | 11.6 (7) | C18—C25—C26—O2 | 5.8 (19) |
| O5—Tb1—N2—C10 | −33.4 (5) | C18—C25—C26—C27 | −173.8 (11) |
| O1—Tb1—N2—C10 | 43.9 (5) | O2—C26—C27—C28 | 25.8 (14) |
| O4—Tb1—N2—C10 | −163.0 (6) | C25—C26—C27—C28 | −154.6 (10) |
| O6—Tb1—N2—C10 | −106.6 (6) | O2—C26—C27—C32 | −154.9 (10) |
| N1—Tb1—N2—C10 | 176.8 (6) | C25—C26—C27—C32 | 24.8 (15) |
| O3—Tb1—O2—C26 | 44.0 (9) | C32—C27—C28—C29 | −1.3 (17) |
| O5—Tb1—O2—C26 | −13.2 (12) | C26—C27—C28—C29 | 178.0 (11) |
| O1—Tb1—O2—C26 | −34.6 (9) | C27—C28—C29—C30 | 0.4 (19) |
| O4—Tb1—O2—C26 | 117.4 (9) | C28—C29—C30—C31 | 2 (2) |
| O6—Tb1—O2—C26 | 169.1 (9) | C29—C30—C31—C32 | −2.8 (19) |
| N2—Tb1—O2—C26 | −104.5 (9) | C28—C27—C32—C31 | 0.2 (18) |
| N1—Tb1—O2—C26 | −160.0 (10) | C26—C27—C32—C31 | −179.2 (11) |
| C1—C2—C3—C4 | 2 (3) | C30—C31—C32—C27 | 2 (2) |
| O2—Tb1—O3—C33 | 43.7 (7) | Tb1—O3—C33—C40 | 24.6 (12) |
| O5—Tb1—O3—C33 | −165.2 (7) | Tb1—O3—C33—C34 | −154.1 (6) |
| O1—Tb1—O3—C33 | 117.4 (7) | O3—C33—C34—C35 | 13.6 (14) |
| O4—Tb1—O3—C33 | −34.1 (7) | C40—C33—C34—C35 | −165.1 (9) |
| O6—Tb1—O3—C33 | −103.0 (7) | O3—C33—C34—C39 | −163.8 (9) |
| N2—Tb1—O3—C33 | 149.5 (6) | C40—C33—C34—C39 | 17.4 (14) |
| N1—Tb1—O3—C33 | −5.1 (9) | C39—C34—C35—C36 | −1.5 (17) |
| C2—C3—C4—C5 | −2 (2) | C33—C34—C35—C36 | −179.0 (10) |
| O2—Tb1—O4—C41 | −53.6 (9) | C34—C35—C36—C37 | −2 (2) |
| O3—Tb1—O4—C41 | 33.7 (8) | C35—C36—C37—C38 | 4 (2) |
| O5—Tb1—O4—C41 | 95.7 (10) | C36—C37—C38—C39 | −2.4 (19) |
| O1—Tb1—O4—C41 | −10.9 (11) | C35—C34—C39—C38 | 3.2 (16) |

| | | | |
|---|---|---|---|
| O6—Tb1—O4—C41 | 155.2 (10) | C33—C34—C39—C38 | −179.4 (9) |
| N2—Tb1—O4—C41 | −149.2 (7) | C37—C38—C39—C34 | −1.3 (17) |
| N1—Tb1—O4—C41 | −131.3 (10) | O3—C33—C40—C41 | 5.3 (15) |
| C1—N1—C5—C4 | −1.9 (17) | C34—C33—C40—C41 | −176.0 (9) |
| Tb1—N1—C5—C4 | 161.9 (8) | Tb1—O4—C41—C40 | −24.9 (14) |
| C1—N1—C5—C6 | 178.1 (9) | Tb1—O4—C41—C42 | 153.9 (6) |
| Tb1—N1—C5—C6 | −18.0 (12) | C33—C40—C41—O4 | −4.4 (16) |
| C3—C4—C5—N1 | 1.8 (17) | C33—C40—C41—C42 | 176.8 (8) |
| C3—C4—C5—C6 | −178.2 (10) | O4—C41—C42—C43 | 18.0 (13) |
| O2—Tb1—O5—C48 | −150.4 (10) | C40—C41—C42—C43 | −163.1 (9) |
| O3—Tb1—O5—C48 | 151.0 (10) | O4—C41—C42—C47 | −162.8 (10) |
| O1—Tb1—O5—C48 | −129.3 (10) | C40—C41—C42—C47 | 16.1 (14) |
| O4—Tb1—O5—C48 | 91.7 (11) | C47—C42—C43—C44 | −2.2 (18) |
| O6—Tb1—O5—C48 | 28.2 (10) | C41—C42—C43—C44 | 177.1 (12) |
| N2—Tb1—O5—C48 | −51.4 (10) | C42—C43—C44—C45 | 1 (2) |
| N1—Tb1—O5—C48 | −15.2 (11) | C43—C44—C45—C46 | −1 (2) |
| C10—N2—C6—C7 | 2.7 (12) | C44—C45—C46—C47 | 2 (2) |
| Tb1—N2—C6—C7 | −157.9 (7) | C45—C46—C47—C42 | −3 (2) |
| C10—N2—C6—C5 | −176.0 (7) | C43—C42—C47—C46 | 3.0 (16) |
| Tb1—N2—C6—C5 | 23.4 (9) | C41—C42—C47—C46 | −176.2 (10) |
| N1—C5—C6—N2 | −3.1 (12) | Tb1—O5—C48—C55 | −23.3 (18) |
| C4—C5—C6—N2 | 176.9 (9) | Tb1—O5—C48—C49 | 157.7 (9) |
| N1—C5—C6—C7 | 178.2 (10) | O5—C48—C49—C54 | 158.3 (12) |
| C4—C5—C6—C7 | −1.8 (14) | C55—C48—C49—C54 | −21 (2) |
| O2—Tb1—O6—C56 | 146.4 (10) | O5—C48—C49—C50 | −25.9 (19) |
| O3—Tb1—O6—C56 | −98.2 (10) | C55—C48—C49—C50 | 155.0 (11) |
| O5—Tb1—O6—C56 | −32.2 (10) | C54—C49—C50—C51 | 0 (2) |
| O1—Tb1—O6—C56 | 2.9 (13) | C48—C49—C50—C51 | −175.8 (15) |
| O4—Tb1—O6—C56 | −162.7 (11) | C49—C50—C51—C52 | −2 (3) |
| N2—Tb1—O6—C56 | 50.8 (10) | C50—C51—C52—C53 | 3 (3) |
| N1—Tb1—O6—C56 | 114.9 (11) | C51—C52—C53—C54 | −1 (2) |
| N2—C6—C7—C8 | −0.9 (15) | C50—C49—C54—C53 | 1 (2) |
| C5—C6—C7—C8 | 177.7 (9) | C48—C49—C54—C53 | 177.1 (13) |
| C6—C7—C8—C9 | −3.4 (16) | C52—C53—C54—C49 | −1 (2) |
| C6—C7—C8—C11 | 175.9 (9) | O5—C48—C55—C56 | 5.6 (18) |
| C7—C8—C9—C10 | 5.5 (16) | C49—C48—C55—C56 | −175.4 (11) |
| C11—C8—C9—C10 | −173.9 (9) | Tb1—O6—C56—C55 | 33.0 (16) |
| C7—C8—C9—C14 | 180.0 (9) | Tb1—O6—C56—C57 | −147.2 (8) |
| C11—C8—C9—C14 | 0.6 (15) | C48—C55—C56—O6 | −11.1 (17) |
| C6—N2—C10—C9 | −0.3 (12) | C48—C55—C56—C57 | 169.2 (10) |
| Tb1—N2—C10—C9 | 160.6 (6) | O6—C56—C57—C58 | −15.3 (14) |
| C8—C9—C10—N2 | −3.9 (14) | C55—C56—C57—C58 | 164.5 (10) |
| C14—C9—C10—N2 | −178.0 (8) | O6—C56—C57—C62 | 164.1 (10) |
| C9—C8—C11—C12 | 0.4 (14) | C55—C56—C57—C62 | −16.1 (15) |
| C7—C8—C11—C12 | −179.0 (10) | C62—C57—C58—C59 | −2.9 (19) |
| C8—C11—C12—C13 | 47.2 (12) | C56—C57—C58—C59 | 176.5 (12) |
| C8—C11—C12—C15 | −50.0 (12) | C57—C58—C59—C60 | 1 (2) |
| C11—C12—C13—C16 | 39.0 (13) | C58—C59—C60—C61 | 2 (2) |

| | | | |
|---|---|---|---|
| C15—C12—C13—C16 | 147.8 (10) | C59—C60—C61—C62 | −3 (2) |
| C11—C12—C13—C17 | 167.7 (10) | C60—C61—C62—C57 | 1 (2) |
| C15—C12—C13—C17 | −83.6 (11) | C58—C57—C62—C61 | 1.9 (18) |
| C11—C12—C13—C14 | −80.8 (10) | C56—C57—C62—C61 | −177.5 (11) |
| C15—C12—C13—C14 | 27.9 (8) | | |