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Borotropic shifting of the hydrotris[3-(2-furyl)-pyrazol-1-yl]borate ligand in high-coordinate lanthanide complexes

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The coordination of hydrotris[3-(2-furyl)pyrazol-1-yl]borate ($Tp^{2\text{-Fu}}$, $C_{21}H_{16}BN_6O_3$) to lanthanide(III) ions is achieved for the first time with the complex $[Ln(Tp^{2\text{-Fu}})_2](BPh_4)\cdot xCH_2Cl_2$ (**1-Ln** has Ln = Ce and x = 2; **1-Dy** has Ln = Dy and x = 1). This was accomplished *via* both hydrous (Ln = Ce) and anhydrous methods (Ln = Dy). When isolating the dysprosium analogue, the filtrate produced a second crop of crystals which were revealed to be the 1,2-borotropic-shifted product $[Dy(\kappa^4\text{-}Tp^{2\text{-Fu}})(\kappa^5\text{-}Tp^{2\text{-Fu}}*)](BPh_4)$ (**2**) {$Tp^{2\text{-Fu}}*$ = hydrobis[3-(2-furyl)pyrazol-1-yl][5-(2-furyl)pyrazol-1-yl]borate}. We conclude that the presence of a strong Lewis acid and a sterically crowded coordination environment are contributing factors for the 1,2-borotropic shifting of scorpionate ligands in conjunction with the size of the conical angle with the scorpionate ligand.

1. Introduction

Since their genesis, scorpionate ligands have been used in coordination chemistry due to their high denticity and charged nature (Trofimenko, 1966). It was not until the 1970s that the first lanthanide complexes featuring scorpionate ligands were synthesized, namely, $LnTp_3$ [Tp = hydrotris(pyrazol-1-yl)borate] complexes (Bagnall *et al.*, 1976), but since then many lanthanide complexes have followed [there are 528 structures in the Cambridge Structural Database (CSD; Groom *et al.*, 2016) as of December 2023]. One such scorpionate that has not yet been used in lanthanide coordination chemistry is hydrotris[3-(2-furyl)pyrazol-1-yl]borate ($Tp^{2\text{-Fu}}$), which bears a resemblance to hydrotris[3-(2-pyridyl)pyrazol-1-yl)borate ($Tp^{2\text{-py}}$), where the 2-pyridyl group has been replaced by the differently coordinating 2-furyl heterocycle (Scheme 1). $Tp^{2\text{-Fu}}$ has been used previously in transition-metal complexation, namely, with Cu (Halcrow *et al.*, 1997) and Zn (Maldonado Calvo *et al.*, 2006); however, the 2-furyl substituents do not partake in any coordination in these transition-metal complexes. The $Tp^{2\text{-py}}$ ligand was heavily used within lanthanide coordination chemistry in the late 1990s and early 2000s by McCleverty and Ward (Amoroso *et al.*, 1994; Jones *et al.*, 1997; Bell *et al.*, 2001; Beeby *et al.*, 2002), where the ligand was exploited for its hexadentate nature as the authors quote 'the cavity is an appropriate size for lanthanide(III) ions' (Jones *et al.*, 1997). In McCleverty and Ward's systems, the 2-pyridyl substituents do coordinate to lanthanide ions, but systematic changes to this functional group were not explored by the authors.

Due to the difference in ring size of the 3-*R*-pyrazole (where *R* = 2-pyridyl or 2-furyl) functional groups, they present a different cavity size and, by extension, conical angles (where the measured conical angle is from the metal centre to the B

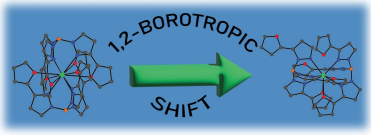


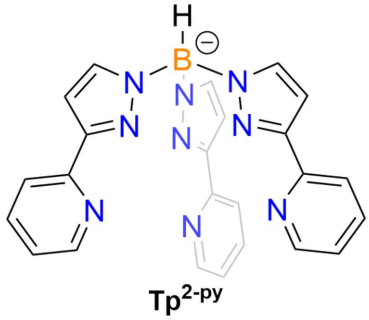
Table 1
Experimental details.

Experiments were carried out at 100 K with Mo $K\alpha$ radiation using a Bruker D8 QUEST diffractometer. Absorption was corrected for by multi-scan methods (*SADABS*; Bruker, 2016). H atoms were treated by a mixture of independent and constrained refinement.

	1-Ce	**1-Dy**	**2**
Crystal data			
Chemical formula	$[Ce(C_{21}H_{16}BN_6O_3)_2]$-$(C_{24}H_{20}B)\cdot 2CH_2Cl_2$	$[Dy(C_{21}H_{16}BN_6O_3)_2]$-$(C_{24}H_{20}B)\cdot 2CH_2Cl_2$	$[Dy(C_{21}H_{16}BN_6O_3)_2](C_{24}H_{20}B)$
M_r	1451.59	1389.05	1304.12
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$
a, b, c (Å)	11.2742 (5), 27.1355 (13), 21.3644 (10)	12.1461 (7), 16.1883 (8), 17.1795 (10)	11.7200 (4), 11.9389 (5), 21.9139 (9)
α, β, γ (°)	90, 90.166 (2), 90	102.659 (2), 103.322 (2), 95.948 (2)	75.579 (2), 76.715 (1), 86.477 (1)
V (Å^3)	6536.0 (5)	3164.6 (3)	2890.2 (2)
Z	4	2	2
μ (mm^{-1})	0.92	1.33	1.36
Crystal size (mm)	0.3 × 0.25 × 0.05	0.3 × 0.2 × 0.05	0.2 × 0.2 × 0.1
Data collection			
T_{min}, T_{max}	0.629, 0.746	0.610, 0.747	0.672, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	596858, 16177, 14693	245023, 12926, 11705	230574, 11804, 10724
R_{int}	0.056	0.058	0.052
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.667	0.625	0.625
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.085, 1.06	0.044, 0.105, 1.08	0.028, 0.066, 1.18
No. of reflections	16177	12926	11804
No. of parameters	855	930	801
No. of restraints	0	14	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.64, −1.42	2.71, −1.74	2.69, −1.00

Computer programs: *APEX3* (Bruker, 2019), *SAINT* (Bruker, 2019), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2019* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

atom of the scorpionate then to the coordinating N atom on the pyrazolyl ring, *i.e.* Ln···B···N_{pz}), and therefore are likely



Tp$^{2\text{-py}}$

Tp$^{2\text{-Fu}}$

Scheme 1

to have different coordination chemistry. It has recently been shown by us (Thomas *et al.*, 2024) that when encapsulating lanthanide ions in a *bis*-Tp$^{2\text{-py}}$ ligand environment, the size of the lanthanide ion dictates the stability of the high-coordinate complexes. The 12-coordinate pseudo-icosahedral complexes ($[Ln(Tp^{2\text{-py}})_2]^+$) exhibit high stability from lanthanum(III) to terbium(III) before the dysprosium(III) analogue converges on a stable 9-coordinate water-introduced complex $[Dy(\kappa^4\text{-}Tp^{2\text{-py}})_2(H_2O)]^+$. Thus, to explore the stability of *bis*-Tp$^{2\text{-Fu}}$ lanthanide complexes, the coordination chemistry of said ligand is presented herein.

2. Experimental

2.1. Synthesis and crystallization

$NaTp^{2\text{-Fu}}$ was synthesized according to literature procedures (Halcrow *et al.*, 1997), with progression of the pyrazolyl substitution tracked by our *in-situ* methods (Thomas *et al.*, 2021). $[Ce(Tp^{2\text{-Fu}})_2](BPh_4)\cdot 2CH_2Cl_2$ (**1-Ce**) was prepared by an adapted literature procedure with analogous ligands (Jones *et al.*, 1997; Thomas *et al.*, 2024), *i.e.* a one-pot salt metathesis reaction in methanol from $CeCl_3\cdot 7H_2O$, $NaTp^{2\text{-Fu}}$ and $NaBPh_4$ at a 1:2:1 loading, where **1-Ce** was recrystallized from CH_2Cl_2/pentane. A similar literature adaptation was used to prepare $[Dy(Tp^{2\text{-Fu}})_2](BPh_4)\cdot CH_2Cl_2$ (**1-Dy**), *i.e.* an anhydrous one-pot salt metathesis reaction in dry tetrahydrofuran (THF) from anhydrous $DyCl_3$, $NaTp^{2\text{-Fu}}$ and $NaBPh_4$ at a 1:2:1 loading, where **1-Dy** was recrystallized from CH_2Cl_2/pentane. After filtering the mother liquor of **1-Dy** under inert conditions, crystals of $[Dy(\kappa^4\text{-}Tp^{2\text{-Fu}})(\kappa^5\text{-}Tp^{2\text{-Fu}}*)](BPh_4)$ (**2**) {$Tp^{2\text{-Fu}}*$ = hydrobis[3-(2-furyl)pyrazol-1-yl][5-(2-furyl)pyrazol-1-yl]borate} were grown.

Table 2
Selected bond distances (Å) and angles (°), and Continuous Shape Measurement (CShM) values for coordination geometries calculated by *SHAPE2.1* (Pinsky *et al.*, 1998).

	1-Ce	**1-Dy**	**2**	
			$Tp^{2\text{-}Fu}$	**$Tp^{2\text{-}Fu}$***
Ln···B	3.865 (3), 3.878 (3)	3.720 (7), 3.740 (6)	3.601 (2)	3.611 (3)
Ln—N_{pz}	2.638 (2)–2.674 (2)	2.489 (4)–2.626 (3)	2.375 (2)–2.558 (2)	2.411 (2)–2.455 (2)
Ln—O_{Fu}	2.809 (2)–2.890 (2)	2.755 (3)–3.181 (3)	2.5417 (17)	2.6400 (18), 2.8420 (18)
Furyl torsion angle	1.8 (3)–7.1 (3)	0.4 (6)–15.2 (6)	3.0 (3), 23.5 (4), 36.7 (6), 149 (1)*	3.0 (3), 6.7 (3), 150.8 (2)
Conical angle	42.45 (6)–43.27 (6)	41.7 (1)–44.6 (1)	41.04 (6)–45.26 (6)	41.74 (7)–42.78 (7)
B···Ln···B	179.30 (5)	173.1 (1)	155.94 (6)	
CShM (geometry)	0.358 (I_c)	1.034 (I_c)	1.422 (CSA)	

Notes: N_{pz} = coordinating pyrazolyl N atom; O^{Fu} = coordinating furyl O atom; furyl torsion angle = angle between pyrazolyl and furyl groups measured from N_{pz} to O_{Fu}; I_c = icosahedral; CSA = capped square antiprism. (*) Two conformations of the furyl group are present in **2** for one pyrazolyl substituent.

Full details of the syntheses are given in the supporting information.

2.2. Single-crystal collection and refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were fixed using the riding model, apart from the borohydride H atoms (on the scorpionate ligands), which were placed based on residual electron density, with bond distances and angles allowed to refine until convergence. *OLEX2* (Dolomanov *et al.*, 2009) was employed for refining data and producing the molecular graphics.

The following disorder was observed. **1-Ce** had large residual electron-density peaks which were removed with a solvent mask and assigned to an extra CH_2Cl_2 molecule. **1-Dy** had a 3-(2-furyl)pyrazole fragment in the lattice that was removed *via* the implantation of a solvent mask using *OLEX2*, correlating to *ca* 0.75 pyrazole units. **1-Dy** also displayed a twisting disorder in the arene rings of the BPh_4^- counter-ion and lattice solvent disorder for the CH_2Cl_2 molecule. Structure **2** has a large unexplained electron-density peak close to a C atom of the BPh_4^- anion. This could not be modelled as disorder and thus may indicate an unresolved problem with the reflection data.

3. Results and discussion

Previous coordination of $Tp^{2\text{-}Fu}$ or its derivatives was achieved with the copper(II) complex [Cu*L*($Tp^{2\text{-}Fu}$)]BF_4 [*L* = 3-(2,5-dimethoxyphenyl)-1-(2-pyridyl)pyrazole] and the zinc(II) complexes [Zn($Tp^{2\text{-}Fu,Me}$)$_2$] and [Zn($Tp^{2\text{-}Fu,Me}$)*R*] {$Tp^{2\text{-}Fu,Me}$ = hydrotris[3-(2-furyl)-5-methylpyrazol-1-yl]borate; *R* = Cl, Br, I, NCS, CH_3CO_2, CF_3CO_2, OH, CH_3OCO_2, SCSOMe, $OPO(ONit)_2$, ONit (*i.e.* 4-nitrophenyl), $S(CH_2)_3COOMe$ or $NHCOCF_3$}. The transition-metal complexes result in short coordination bonds with the coordinating pyrazolyl N atom [N_{pz}; Cu—N_{pz} = 1.985 (4)–2.241 (4) Å and Zn—N_{pz} = 2.011 (3)–2.257 (6) Å] and, for the *bis*-capped complexes, the 2-furyl groups point away from the metal centres. Since the 3-*R*-substituted scorpionate ligands that employ coordinating functional groups in the past have been shown to coordinate to lanthanide ions, we envisioned the same would be true for the $Tp^{2\text{-}Fu}$ ligand.

The syntheses of **1-Ce** and **1-Dy** were achieved *via* adaptations of literature procedures (Jones *et al.*, 1997; Thomas *et al.*, 2024). Use of hydrated $CeCl_3$ and $NaTp^{2\text{-}Fu}$ stirred in methanol before the addition of a methanolic solution of $NaBPh_4$ produces a precipitate of **1-Ce**, which was further recrystallized from layering a CH_2Cl_2 solution of **1-Ce** with pentane. **1-Ce** is air-stable, does not decompose over time and has been stored open to air for over a year. Due to the size of

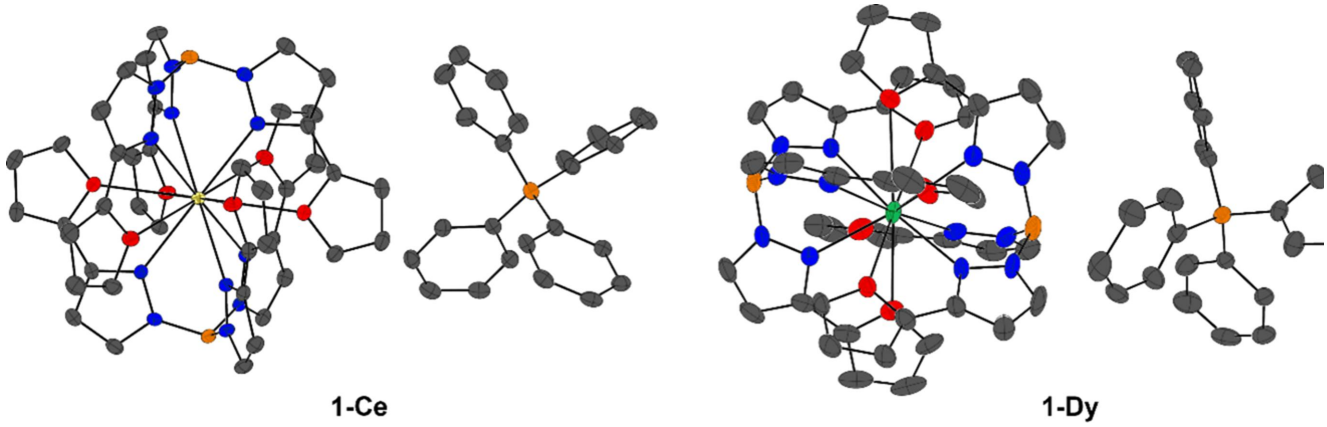


Figure 1
Solid-state structures of **1-Ln**, where Ln = Ce (left) and Dy (right), shown with 50% probability displacement ellipsoids. Colour codes: Dy^{III} turquoise, Ce^{III} cream, O red, N blue, C grey and B orange. H atoms have been omitted for clarity.

dysprosium(III) ions, we synthesized **1-Dy** by anhydrous routes to encourage the formation of the pseudo-icosahedral crystal field, as the use of hydrated methods for analogous ligands results in the rearrangement of the complex to one with a lower coordination number (Thomas *et al.*, 2024). Thus, anhydrous $DyCl_3$, $NaTp^{2\text{-Fu}}$ and $NaBPh_4$ were all stirred in THF before the solvent was removed *in vacuo*, and the crude material was dissolved in CH_2Cl_2, filtered and layered with pentane to produce single crystals of **1-Dy**.

The solid-state structures of the cations in **1-Ce** and **1-Dy** are presented in Fig. 1, with selected data summarized in Table 2. The cations in **1-Ce** and **1-Dy** both produced pseudo-icosahedral (I_c) crystal fields where the N_{pz} atoms are axial, akin to cyclopentadienyl (Cp) donations being axial, and with the coordinating O atoms from the furyl groups (O_{Fu}) forming an equatorial 'belt' with respect to the N_{pz}. Due to the size differences between Ce^{III} and Dy^{III}, most of the coordination bonds are shorter in **1-Dy** owing to the scorpionate ligand residing closer to the lanthanide centre (see Table 2 for B···Ln distance). Few Ln—O_{Fu} distances are larger in **1-Dy** since the furyl group extends past the plane that divides the molecule in half, and there are larger torsion angles between the pyrazolyl and furyl groups within each borate substituent (torsion angle is measured from N_{pz} to O_{Fu}, including the two C atoms between the N_{pz} and O_{Fu} atoms).

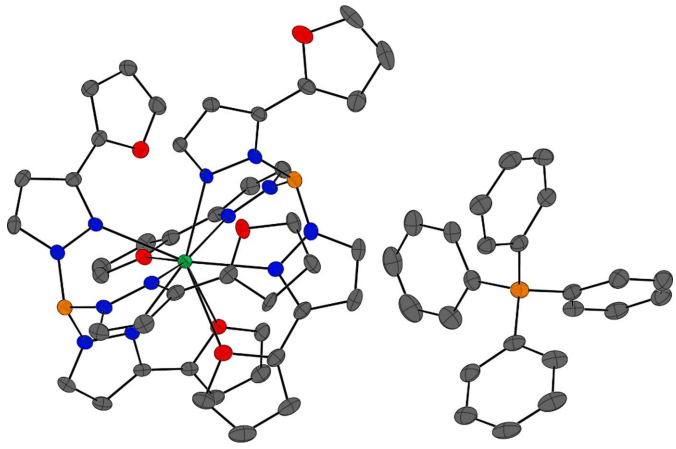


Figure 3
Solid-state structure of **2**, shown with 50% probability displacement ellipsoids. The colour codes are as in Fig. 1 and H atoms have been omitted for clarity. Only one conformation of the disordered furyl ring is shown, where the furyl torsion angle is 36.7 (6)°.

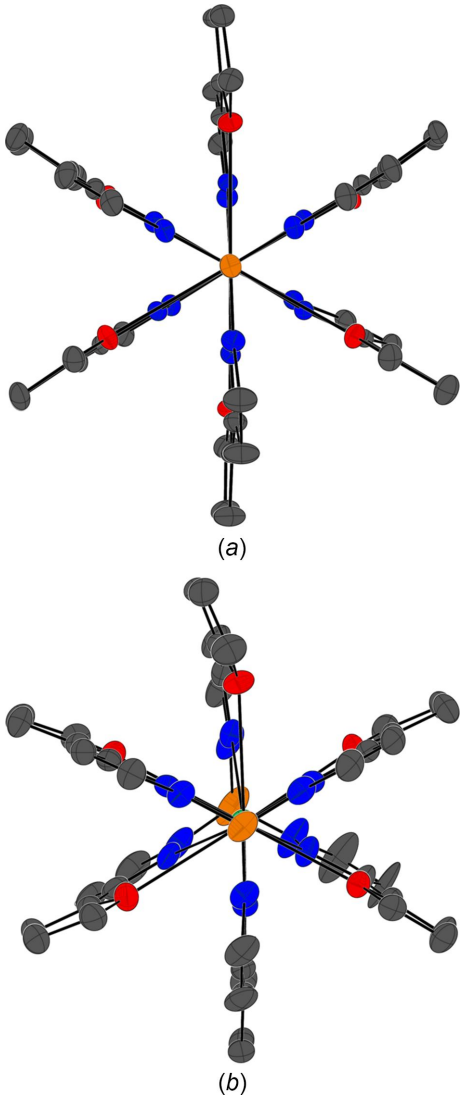


Figure 2
View from the pseudo-B···B axis in **1-Ln**, where Ln is (*a*) Ce and (*b*) Dy.

The coordination distances and measured angles in **1-Dy** have larger ranges than those observed in **1-Ce**, suggesting that the structure is sterically crowded. Steric crowding is most evident by the deviation of the B···Ln···B angle from being approximately linear in **1-Ce** to 173.1 (1)° in **1-Dy**. Viewing the cations in **1-Ln** from the pseudo-B···B axis (Fig. 2) brings light to said strain seen in **1-Dy**, where it can be thought that there is a loss of the psudeo-S_6 axis that is more evident in **1-Ce**. These axial perspectives make it easier to visualize the larger torsion angles of the furyl groups that are present in **1-Dy**.

To investigate the strain seen in **1-Dy**, Continuous Shape Measurements (CShM) were performed employing *SHAPE2.1* (Pinsky *et al.*, 1998) to measure the distortion of the crystal field from a regular I_c (Table 2). The results of the CShM not only show that the crystal field in **1-Dy** deviates more from I_c than in **1-Ce**, but that **1-Dy** also exhibits the highest CShM value seen in pseudo-I_c *bis*-scorpionate-encapsulated lanthanide complexes (Thomas *et al.*, 2024). The high CShM value is no surprise given the strain in the cation present in Fig. 2.

Upon filtering off the mother liquor to isolate **1-Dy**, the recrystallization of 1,2-borotropic-shifted complex **2** occurred within the filtrate over a period of several days. Borotropic shifting in scorpionate ligands has been reported previously and occurs due to the presence of a large substituent on the third position of the pyrazolyl group, *i.e.* isopropyl (Trofimenko *et al.*, 1989; Cano *et al.*, 1990; White *et al.*, 2009), *tert*-butyl (Chisholm *et al.*, 1996), phenyl (Zhao *et al.*, 2007; Cui *et al.*, 2010) and mesityl (Rheingold *et al.*, 1993), causing steric congestion around a metal centre and hence undergoes rearrangement to reduce the steric crowding around it. One

example that is noteworthy is [Nd(Tp^{Ph}*)(THF)(μ-PC_6H_3-2,6-$^iPr_2$)]$_2$ [Tp^{Ph}* = hydrobis(3-phenylpyrazol-1-yl)(5-phenylpyrazol-1-yl)borate] (Cui *et al.*, 2010), where the aryl substituents on the bridging phosphinidenes cause steric congestion around the neodymium(III) centre; thus, the scorpionate undergoes a 1,2-borotropic shift. We believe that for borotropic shifting to occur there are a few conditions that need to be met: sufficient steric crowding around the metal centre, the conical angle of the scorpionate needs to be small and the metal centre needs to possess a certain Lewis acidity. The size of the conical angle is dependent on which scorpionate is used and must be relatively small for said scorpionate in order for shifting to occur. For the case of **1-Dy**, these conditions are met, whereas for **1-Ce**, the Lewis acidity is lower for the metal centre and the conical angles are slightly larger (Table 2). The Lewis acidity of lanthanides is a direct consequence of ion size; thus, as the size of cerium(III) is larger [*cf.* dysprosium(III)], the $Tp^{2\text{-Fu}}$ ligands sit further away from the metal centre and are not sterically congested.

The solid-state structure of the cation [Dy(κ^4-$Tp^{2\text{-Fu}}$)(κ^5-$Tp^{2\text{-Fu}}$*)]$^+$ in **2** is shown in Fig. 3, with the structural data presented in Table 2. One of the scorpionate ligands maintains its structure but resides much closer to the dysprosium(III) centre than in **1-Dy**, with a B···Dy distance of 3.601 (2) Å and a Dy—N_{pz} range of 2.375 (2)–2.558 (2) Å. This ligand also loses denticity adopting a κ^4-binding mode, where two of the 2-furyl groups do not coordinate to the metal centre likely due to steric crowding, resulting in significantly larger furyl torsion angles of 23.5 (4) and 36.7 (6)°. The second furyl substituent in this ligand is disordered over two sites, where the additional furyl torsion angle is 149 (1)°, thus pointing away from the dysprosium centre (Fig. S4 in the supporting information). The one 2-furyl substituent in **2** that does coordinate has a shorter coordination bond of 2.542 (2) Å in comparison with the 2-furyl substituents in **1-Dy**. The borotropic-shifted scorpionate $Tp^{2\text{-Fu}}$* in **2** also resides much closer to the dysprosium(III) centre [Dy···B = 3.613 (4) Å and Dy—N_{pz} = 2.411 (2)–2.455 (2) Å] than in **1-Dy**, likely owing to the less sterically congested coordination environment. Due to the borotropic shift, one pyrazolyl substituent of the ligand is substituted in the 5-position, with the O_{Fu} atom pointing away from the metal centre; thus, the denticity of the ligand is reduced to κ^5, as the remaining coordination bonds are maintained. The overall coordination number of **2** reduces to nine given the denticity of each ligand, with a capped square antiprismatic (CSA) crystal field environment. The coordinating 2-furyl in $Tp^{2\text{-Fu}}$* also present shorter Dy—O_{Fu} coordination bonds of 2.6400 (19) and 2.8418 (19) Å. Overall, the borotropic shifting of the $Tp^{2\text{-Fu}}$ ligands produces a complex where the scorpionate ligands bind 'tighter' as the ligands reside closer to the dysprosium(III), which gives rise to a smaller nonlinear B···Dy···B angle of 155.94 (8)°.

4. Conclusions

Through the synthesis of an early and mid-lanthanide *bis*-$Tp^{2\text{-Fu}}$ complex, we have demonstrated that 1,2-borotropic shifting of scorpionate ligands is likely dependent on the size, and hence Lewis acidity, of the lanthanide ion and how close the 3-*R*-substituted scorpionate ligands reside, as seen in the literature. The hydrate synthetic route of **1-Ce** and air-stability of this complex aid this argument, while the anhydrous synthesis of **1-Dy** still results in the isolation of the more stable borotropic-shifted **2**.

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References

Amoroso, A. J., Thompson, A. M. C., Jeffery, J. C., Jones, P. L., McCleverty, J. A. & Ward, M. D. (1994). *J. Chem. Soc. Chem. Commun.* pp. 2751–2752.
Bagnall, K. W., Tempest, A. C., Takats, J. & Masino, A. P. (1976). *Inorg. Nucl. Chem. Lett.* **12**, 555–557.
Beeby, A., Burton-Pye, B. P., Faulkner, S., Motson, G. R., Jeffery, J. C., McCleverty, J. A. & Ward, M. D. (2002). *J. Chem. Soc. Dalton Trans.* pp. 1923–1928.
Bell, Z. R., Motson, G. R., Jeffery, J. C., McCleverty, J. A. & Ward, M. D. (2001). *Polyhedron*, **20**, 2045–2053.
Bruker (2016). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2019). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cano, M., Heras, J. V., Trofimenko, S., Monge, A., Gutierrez, E., Jones, C. J. & McCleverty, J. A. (1990). *J. Chem. Soc. Dalton Trans.* pp. 3577–3582.
Chisholm, M. H., Eilerts, N. W. & Huffman, J. C. (1996). *Inorg. Chem.* **35**, 445–450.
Cui, P., Chen, Y. & Borzov, M. V. (2010). *Dalton Trans.* **39**, 6886–6890.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Halcrow, M. A., McInnes, E. J. L., Mabbs, F. E., Scowen, I. J., McPartlin, M., Powell, H. R. & Davies, J. E. (1997). *J. Chem. Soc. Dalton Trans.* pp. 4025–4036.
Jones, P. L., Amoroso, A. J., Jeffery, J. C., McCleverty, J. A., Psillakis, E., Rees, L. H. & Ward, M. D. (1997). *Inorg. Chem.* **36**, 10–18.
Maldonado Calvo, J. A. & Vahrenkamp, H. (2006). *Inorg. Chim. Acta*, **12**, 4079–4086.
Pinsky, M. & Avnir, D. (1998). *Inorg. Chem.* **37**, 5575–5582.
Rheingold, A. L., White, C. B. & Trofimenko, S. (1993). *Inorg. Chem.* **32**, 3471–3477.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Thomas, J. R., Giansiracusa, M. J., Mole, R. A. & Sulway, S. A. (2024). *Cryst. Growth Des.* **24**, 573–583.
Thomas, J. R. & Sulway, S. A. (2021). *RSC Adv.* **11**, 16158–16160.
Trofimenko, S. (1966). *J. Am. Chem. Soc.* **88**, 1842–1844.
Trofimenko, S., Calabrese, J. C., Domaille, P. J. & Thompson, J. S. (1989). *Inorg. Chem.* **28**, 1091–1101.

White, J. M., Ng, V. W. L., Clarke, D. C., Smith, P. D., Taylor, M. K. & Young, X. G. (2009). *Inorg. Chim. Acta*, **362**, 4570–4577.

Zhao, N., Van Stipdonk, M. J., Bauer, C., Campana, C. & Eichhorn, D. M. (2007). *Inorg. Chem.* **46**, 8662–8667.

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Borotropic shifting of the hydrotris[3-(2-furyl)pyrazol-1-yl]borate ligand in high-coordinate lanthanide complexes

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Computing details

Bis{hydrotris[3-(2-furyl)pyrazol-1-yl]borato}cerium(III) tetraphenylborate dichloromethane disolvate (1Ce)

Crystal data

$[Ce(C_{21}H_{16}BN_6O_3)_2](C_{24}H_{20}B)\cdot 2CH_2Cl_2$
M_r = 1451.59
Monoclinic, $P2_1/c$
a = 11.2742 (5) Å
b = 27.1355 (13) Å
c = 21.3644 (10) Å
β = 90.166 (2)°
V = 6536.0 (5) Å^3
Z = 4
$F(000)$ = 2948
D_x = 1.475 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9697 reflections
θ = 2.2–30.6°
μ = 0.92 mm^{-1}
T = 100 K
Block, clear colourless
0.3 × 0.25 × 0.05 mm

Data collection

Bruker D8 QUEST diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.629, T_{max} = 0.746
596858 measured reflections
16177 independent reflections
14693 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 28.3°, θ_{min} = 1.8°
h = −15→15
k = −36→36
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.06
16177 reflections
855 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 12.1467P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 1.64 e Å^{-3}
$\Delta\rho_{min}$ = −1.42 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data were collected on a Bruker D8 QUEST diffractometer at 100 K, fitted with a CCD area detector employing a mirror-monochromatic Mo *Kα* radiation source (λ = 0.71073 Å). Integration and scaling data of collections were analysed using *APEX3* software. All data was collected with exposures times of 10 s with 1° frame sweeps on ω and φ scans. Multi-scan absorption corrections were used for all compounds. Data was solved in *APEX3* software by intrinsic phasing methods using *SHELXL2019* (Sheldrick, 2015*b*). Refinement of the crystal data was carried out using least-squares refinement methods employed by *SHELXT* (Sheldrick, 2015*a*), with all non-H atoms having anisotropic displacement parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ce1	0.53330 (2)	0.76013 (2)	0.42575 (2)	0.01307 (4)
Cl2	−0.06877 (7)	0.85783 (3)	0.73572 (4)	0.04465 (17)
Cl1	0.10738 (9)	0.88399 (5)	0.64384 (5)	0.0665 (3)
Cl3	0.59851 (12)	1.03969 (4)	0.33400 (7)	0.0916 (5)
Cl4	0.76490 (17)	0.99847 (6)	0.42623 (9)	0.1081 (5)
O2	0.35199 (13)	0.70166 (5)	0.47675 (7)	0.0182 (3)
O6	0.71650 (14)	0.82000 (6)	0.37269 (7)	0.0202 (3)
O3	0.47052 (14)	0.82561 (6)	0.32425 (7)	0.0203 (3)
O5	0.29552 (13)	0.79900 (6)	0.42512 (7)	0.0206 (3)
O4	0.59703 (14)	0.69429 (6)	0.52663 (7)	0.0198 (3)
O1	0.77182 (13)	0.72313 (6)	0.42660 (7)	0.0205 (3)
N4	0.44323 (15)	0.78050 (6)	0.53662 (8)	0.0153 (3)
N10	0.37076 (15)	0.72760 (6)	0.34552 (8)	0.0152 (3)
N12	0.62544 (15)	0.74052 (6)	0.31423 (8)	0.0156 (3)
N3	0.46896 (15)	0.81907 (7)	0.57524 (8)	0.0179 (3)
N11	0.59512 (15)	0.70306 (7)	0.27473 (8)	0.0166 (3)
N7	0.54252 (15)	0.63865 (6)	0.35333 (8)	0.0166 (3)
N1	0.68313 (16)	0.83167 (7)	0.54746 (8)	0.0184 (3)
N8	0.55777 (15)	0.66421 (6)	0.40770 (8)	0.0155 (3)
N9	0.38172 (15)	0.68953 (6)	0.30432 (8)	0.0156 (3)
N6	0.51236 (15)	0.85745 (6)	0.44212 (8)	0.0164 (3)
N2	0.69552 (15)	0.79433 (7)	0.50530 (8)	0.0169 (3)
N5	0.52418 (17)	0.88323 (7)	0.49664 (9)	0.0200 (4)
C43	0.06132 (18)	0.89895 (8)	0.17425 (10)	0.0185 (4)
C44	0.12582 (19)	0.86701 (8)	0.21334 (10)	0.0214 (4)
H44	0.181588	0.880806	0.241783	0.026*
C55	−0.04179 (19)	0.98964 (8)	0.16678 (10)	0.0212 (4)
C11	0.31213 (18)	0.71052 (8)	0.53672 (9)	0.0162 (4)
C60	−0.0426 (2)	1.03965 (8)	0.14950 (11)	0.0229 (4)
H60	0.030038	1.054708	0.137768	0.028*
C31	0.25556 (18)	0.74013 (7)	0.34474 (10)	0.0166 (4)
C1	0.7871 (2)	0.83969 (9)	0.57752 (11)	0.0244 (4)
H1	0.800569	0.863904	0.608870	0.029*
C14	0.29604 (19)	0.65888 (8)	0.45727 (10)	0.0196 (4)
H14	0.306617	0.643753	0.417579	0.024*
C48	−0.01810 (19)	0.87551 (9)	0.13278 (11)	0.0222 (4)
H48	−0.062336	0.895213	0.104320	0.027*

C49	0.14511 (19)	0.97993 (8)	0.23690 (11)	0.0214 (4)
C13	0.22461 (19)	0.64184 (8)	0.50263 (11)	0.0210 (4)
H13	0.176108	0.613253	0.500634	0.025*
C39	0.75964 (18)	0.80965 (8)	0.31363 (10)	0.0180 (4)
C24	0.59757 (18)	0.63093 (8)	0.44955 (10)	0.0179 (4)
C23	0.6093 (2)	0.58437 (8)	0.42234 (11)	0.0242 (4)
H23	0.636253	0.554835	0.441540	0.029*
C22	0.5729 (2)	0.59102 (8)	0.36158 (11)	0.0221 (4)
H22	0.569609	0.566109	0.330380	0.027*
C61	0.17096 (19)	0.96765 (8)	0.11149 (11)	0.0201 (4)
C12	0.23540 (19)	0.67482 (8)	0.55437 (11)	0.0212 (4)
H12	0.196323	0.672211	0.593566	0.025*
C62	0.1330 (2)	0.98525 (8)	0.05304 (11)	0.0224 (4)
H62	0.052945	0.995563	0.048488	0.027*
C10	0.35885 (18)	0.75440 (8)	0.56584 (10)	0.0168 (4)
C41	0.8471 (2)	0.87829 (9)	0.34764 (12)	0.0267 (5)
H41	0.896181	0.906686	0.349751	0.032*
C29	0.27493 (19)	0.67854 (8)	0.27907 (10)	0.0190 (4)
H29	0.260046	0.653248	0.249325	0.023*
C42	0.7723 (2)	0.86261 (8)	0.39207 (11)	0.0234 (4)
H42	0.759601	0.878490	0.431110	0.028*
C45	0.1117 (2)	0.81600 (8)	0.21227 (11)	0.0244 (4)
H45	0.157896	0.795914	0.239394	0.029*
C63	0.2080 (2)	0.98827 (8)	0.00121 (11)	0.0243 (4)
H63	0.178718	1.000720	−0.037411	0.029*
C30	0.19140 (19)	0.70996 (8)	0.30348 (10)	0.0203 (4)
H30	0.108883	0.711003	0.294442	0.024*
C28	0.6221 (2)	0.70062 (9)	0.58943 (10)	0.0233 (4)
H28	0.613450	0.730680	0.611756	0.028*
C46	0.0304 (2)	0.79439 (9)	0.17175 (11)	0.0257 (5)
H46	0.019352	0.759688	0.171380	0.031*
C64	0.3253 (2)	0.97306 (8)	0.00614 (12)	0.0256 (5)
H64	0.376465	0.974561	−0.029061	0.031*
C17	0.4756 (2)	0.89038 (8)	0.39919 (10)	0.0208 (4)
C3	0.80888 (18)	0.77949 (8)	0.50991 (10)	0.0190 (4)
C26	0.6611 (2)	0.62221 (9)	0.56522 (11)	0.0244 (4)
H26	0.684787	0.588699	0.568411	0.029*
C59	−0.1455 (2)	1.06798 (9)	0.14887 (11)	0.0266 (5)
H59	−0.141724	1.101705	0.137095	0.032*
C38	0.71046 (18)	0.76610 (8)	0.28457 (9)	0.0165 (4)
C27	0.6605 (2)	0.65793 (9)	0.61436 (11)	0.0255 (5)
H27	0.682912	0.652557	0.656705	0.031*
C56	−0.1523 (2)	0.97029 (9)	0.18375 (13)	0.0313 (5)
H56	−0.156601	0.936764	0.196364	0.038*
C65	0.3665 (2)	0.95570 (9)	0.06310 (12)	0.0266 (5)
H65	0.446673	0.945369	0.067248	0.032*
C21	0.4523 (2)	0.81892 (9)	0.26069 (10)	0.0233 (4)
H21	0.455687	0.788082	0.239727	0.028*

C15	0.4944 (3)	0.93071 (9)	0.48774 (13)	0.0322 (5)
H15	0.495224	0.955695	0.518894	0.039*
C66	0.2906 (2)	0.95337 (8)	0.11437 (12)	0.0239 (4)
H66	0.321164	0.941577	0.153056	0.029*
C37	0.7362 (2)	0.74517 (9)	0.22626 (10)	0.0214 (4)
H37	0.792598	0.756030	0.196337	0.026*
C40	0.8393 (2)	0.84445 (9)	0.29651 (11)	0.0245 (4)
H40	0.881625	0.846050	0.258171	0.029*
C32	0.21357 (18)	0.77990 (8)	0.38371 (10)	0.0188 (4)
C8	0.4013 (2)	0.81684 (9)	0.62712 (10)	0.0232 (4)
H8	0.402915	0.839777	0.660706	0.028*
C36	0.66117 (19)	0.70533 (9)	0.22213 (10)	0.0218 (4)
H36	0.656560	0.683048	0.187915	0.026*
C47	−0.0344 (2)	0.82452 (9)	0.13181 (11)	0.0247 (5)
H47	−0.090201	0.810357	0.103656	0.030*
C9	0.3293 (2)	0.77586 (9)	0.62349 (10)	0.0238 (4)
H9	0.272774	0.764718	0.653173	0.029*
C50	0.2257 (2)	1.01920 (9)	0.23666 (12)	0.0270 (5)
H50	0.249388	1.032596	0.197561	0.032*
C25	0.62125 (18)	0.64566 (8)	0.51297 (10)	0.0184 (4)
C2	0.8701 (2)	0.80713 (10)	0.55530 (11)	0.0264 (5)
H2	0.950661	0.803979	0.567778	0.032*
C58	−0.2529 (2)	1.04738 (10)	0.16526 (13)	0.0331 (6)
H58	−0.323412	1.066571	0.164471	0.040*
C18	0.45732 (19)	0.87548 (8)	0.33518 (10)	0.0204 (4)
C54	0.1132 (2)	0.96298 (10)	0.29663 (12)	0.0316 (5)
H54	0.057273	0.936898	0.299602	0.038*
B3	0.0834 (2)	0.95887 (9)	0.17209 (12)	0.0192 (4)
C7	0.8289 (2)	0.68616 (9)	0.39408 (11)	0.0251 (5)
H7	0.795216	0.667851	0.360563	0.030*
C4	0.85120 (19)	0.73990 (8)	0.47085 (10)	0.0205 (4)
C20	0.4292 (2)	0.86223 (10)	0.23298 (11)	0.0286 (5)
H20	0.414126	0.867469	0.189718	0.034*
C16	0.4625 (3)	0.93712 (9)	0.42611 (13)	0.0336 (6)
H16	0.437332	0.966644	0.406222	0.040*
C5	0.9543 (2)	0.71449 (10)	0.46639 (12)	0.0298 (5)
H5	1.023302	0.718863	0.491427	0.036*
C35	0.2377 (2)	0.83537 (9)	0.45824 (11)	0.0252 (5)
H35	0.272587	0.854812	0.490372	0.030*
C51	0.2727 (2)	1.03948 (10)	0.29135 (14)	0.0340 (6)
H51	0.327314	1.066064	0.288899	0.041*
C19	0.4316 (2)	0.89904 (9)	0.28091 (12)	0.0307 (5)
H19	0.417846	0.933338	0.275695	0.037*
C67	0.0138 (3)	0.90635 (12)	0.70285 (14)	0.0401 (6)
H67A	−0.040844	0.931277	0.685049	0.048*
H67B	0.061893	0.922454	0.735855	0.048*
C57	−0.2564 (2)	0.99824 (11)	0.18290 (15)	0.0389 (6)
H57	−0.329604	0.983539	0.194423	0.047*

C53	0.1598 (3)	0.98265 (11)	0.35184 (13)	0.0410 (7)
H53	0.136335	0.969655	0.391192	0.049*
C33	0.1084 (2)	0.80354 (9)	0.39004 (12)	0.0289 (5)
H33	0.037790	0.797547	0.366914	0.035*
C34	0.1250 (2)	0.83929 (10)	0.43843 (13)	0.0313 (5)
H34	0.067033	0.861640	0.453720	0.038*
C52	0.2400 (3)	1.02102 (11)	0.34920 (14)	0.0377 (6)
H52	0.272393	1.034557	0.386536	0.045*
C6	0.9390 (2)	0.67988 (10)	0.41674 (12)	0.0317 (5)
H6	0.996029	0.656731	0.402423	0.038*
B2	0.5020 (2)	0.66421 (9)	0.29300 (10)	0.0167 (4)
B1	0.5633 (2)	0.85762 (9)	0.55766 (11)	0.0185 (4)
C68	0.7129 (5)	0.99680 (17)	0.3474 (3)	0.0855 (16)
H68A	0.779701	1.003923	0.318874	0.103*
H68B	0.683409	0.963266	0.337840	0.103*
H1A	0.572 (2)	0.8856 (10)	0.5950 (13)	0.022 (7)*
H2A	0.495 (2)	0.6368 (10)	0.2541 (13)	0.023 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.01370 (6)	0.01361 (6)	0.01191 (6)	−0.00026 (4)	0.00097 (4)	−0.00070 (4)
Cl2	0.0421 (4)	0.0414 (4)	0.0504 (4)	0.0011 (3)	−0.0054 (3)	0.0101 (3)
Cl1	0.0564 (5)	0.0932 (8)	0.0499 (5)	0.0007 (5)	0.0127 (4)	−0.0089 (5)
Cl3	0.0948 (9)	0.0524 (6)	0.1281 (11)	0.0308 (6)	0.0570 (8)	0.0230 (6)
Cl4	0.1370 (14)	0.0737 (8)	0.1137 (12)	−0.0045 (9)	0.0172 (10)	−0.0075 (8)
O2	0.0216 (7)	0.0174 (7)	0.0155 (7)	−0.0051 (6)	0.0038 (5)	−0.0022 (5)
O6	0.0209 (7)	0.0217 (7)	0.0182 (7)	−0.0052 (6)	0.0047 (6)	−0.0022 (6)
O3	0.0257 (8)	0.0182 (7)	0.0169 (7)	0.0024 (6)	−0.0023 (6)	0.0012 (6)
O5	0.0172 (7)	0.0207 (7)	0.0238 (8)	0.0021 (6)	−0.0006 (6)	−0.0041 (6)
O4	0.0240 (7)	0.0203 (7)	0.0151 (7)	0.0032 (6)	−0.0024 (6)	−0.0001 (6)
O1	0.0162 (7)	0.0246 (8)	0.0205 (7)	0.0030 (6)	−0.0003 (6)	−0.0036 (6)
N4	0.0167 (8)	0.0151 (8)	0.0143 (7)	−0.0008 (6)	0.0011 (6)	−0.0024 (6)
N10	0.0154 (8)	0.0156 (8)	0.0145 (8)	0.0001 (6)	−0.0004 (6)	0.0003 (6)
N12	0.0168 (8)	0.0165 (8)	0.0136 (8)	0.0005 (6)	0.0021 (6)	0.0001 (6)
N3	0.0185 (8)	0.0190 (8)	0.0161 (8)	−0.0015 (6)	0.0018 (6)	−0.0040 (6)
N11	0.0173 (8)	0.0198 (8)	0.0128 (7)	0.0001 (6)	0.0019 (6)	−0.0018 (6)
N7	0.0187 (8)	0.0150 (8)	0.0160 (8)	0.0013 (6)	0.0011 (6)	−0.0025 (6)
N1	0.0182 (8)	0.0218 (9)	0.0153 (8)	−0.0042 (7)	−0.0002 (6)	−0.0026 (7)
N8	0.0166 (8)	0.0166 (8)	0.0133 (7)	0.0013 (6)	0.0006 (6)	0.0006 (6)
N9	0.0165 (8)	0.0171 (8)	0.0132 (7)	−0.0016 (6)	−0.0010 (6)	0.0004 (6)
N6	0.0175 (8)	0.0157 (8)	0.0161 (8)	−0.0009 (6)	0.0010 (6)	−0.0004 (6)
N2	0.0165 (8)	0.0191 (8)	0.0150 (8)	−0.0008 (6)	−0.0002 (6)	−0.0015 (6)
N5	0.0246 (9)	0.0150 (8)	0.0205 (9)	−0.0006 (7)	0.0000 (7)	−0.0025 (7)
C43	0.0146 (9)	0.0201 (10)	0.0208 (10)	0.0000 (7)	0.0045 (7)	0.0015 (8)
C44	0.0199 (10)	0.0228 (10)	0.0216 (10)	0.0000 (8)	0.0015 (8)	0.0019 (8)
C55	0.0198 (10)	0.0221 (10)	0.0216 (10)	0.0031 (8)	0.0018 (8)	0.0004 (8)
C11	0.0155 (9)	0.0187 (9)	0.0145 (9)	0.0014 (7)	0.0031 (7)	−0.0002 (7)

C60	0.0226 (10)	0.0215 (10)	0.0247 (11)	0.0009 (8)	0.0003 (8)	−0.0009 (8)
C31	0.0156 (9)	0.0178 (9)	0.0164 (9)	−0.0010 (7)	0.0003 (7)	0.0039 (7)
C1	0.0225 (10)	0.0316 (12)	0.0191 (10)	−0.0066 (9)	−0.0038 (8)	−0.0033 (9)
C14	0.0219 (10)	0.0147 (9)	0.0223 (10)	−0.0018 (8)	−0.0007 (8)	−0.0028 (8)
C48	0.0158 (9)	0.0263 (11)	0.0245 (11)	0.0026 (8)	0.0009 (8)	0.0000 (9)
C49	0.0188 (10)	0.0204 (10)	0.0251 (11)	0.0013 (8)	0.0007 (8)	0.0008 (8)
C13	0.0189 (10)	0.0160 (9)	0.0281 (11)	−0.0022 (8)	0.0006 (8)	0.0008 (8)
C39	0.0150 (9)	0.0209 (10)	0.0182 (9)	0.0014 (7)	0.0030 (7)	0.0021 (8)
C24	0.0181 (9)	0.0158 (9)	0.0197 (10)	0.0017 (7)	−0.0001 (7)	0.0023 (7)
C23	0.0293 (11)	0.0172 (10)	0.0262 (11)	0.0048 (8)	−0.0018 (9)	0.0002 (8)
C22	0.0236 (10)	0.0170 (10)	0.0256 (11)	0.0036 (8)	−0.0005 (8)	−0.0029 (8)
C61	0.0198 (10)	0.0163 (9)	0.0242 (10)	−0.0006 (8)	0.0022 (8)	0.0009 (8)
C12	0.0188 (10)	0.0225 (10)	0.0224 (10)	−0.0022 (8)	0.0058 (8)	0.0014 (8)
C62	0.0213 (10)	0.0214 (10)	0.0245 (11)	0.0005 (8)	0.0011 (8)	−0.0011 (8)
C10	0.0149 (9)	0.0195 (9)	0.0161 (9)	0.0000 (7)	0.0022 (7)	0.0008 (7)
C41	0.0214 (10)	0.0230 (11)	0.0358 (13)	−0.0053 (9)	0.0064 (9)	−0.0005 (9)
C29	0.0199 (10)	0.0203 (10)	0.0168 (9)	−0.0053 (8)	−0.0025 (7)	0.0021 (8)
C42	0.0214 (10)	0.0214 (10)	0.0275 (11)	−0.0046 (8)	0.0007 (8)	−0.0040 (9)
C45	0.0262 (11)	0.0214 (10)	0.0255 (11)	0.0039 (8)	0.0057 (9)	0.0054 (8)
C63	0.0297 (11)	0.0214 (10)	0.0219 (10)	−0.0034 (9)	0.0017 (9)	−0.0030 (8)
C30	0.0164 (9)	0.0234 (10)	0.0210 (10)	−0.0034 (8)	−0.0026 (8)	0.0030 (8)
C28	0.0251 (11)	0.0309 (12)	0.0139 (9)	0.0010 (9)	−0.0026 (8)	−0.0016 (8)
C46	0.0248 (11)	0.0204 (10)	0.0320 (12)	−0.0021 (8)	0.0128 (9)	−0.0013 (9)
C64	0.0285 (11)	0.0191 (10)	0.0292 (12)	−0.0056 (9)	0.0105 (9)	−0.0068 (9)
C17	0.0233 (10)	0.0167 (9)	0.0223 (10)	0.0005 (8)	−0.0009 (8)	0.0025 (8)
C3	0.0151 (9)	0.0255 (10)	0.0163 (9)	−0.0020 (8)	−0.0014 (7)	0.0020 (8)
C26	0.0260 (11)	0.0235 (11)	0.0236 (11)	0.0004 (9)	−0.0045 (9)	0.0064 (9)
C59	0.0297 (12)	0.0228 (11)	0.0274 (11)	0.0066 (9)	−0.0014 (9)	−0.0004 (9)
C38	0.0138 (9)	0.0214 (10)	0.0142 (9)	0.0013 (7)	0.0025 (7)	0.0033 (7)
C27	0.0245 (11)	0.0344 (12)	0.0175 (10)	−0.0022 (9)	−0.0036 (8)	0.0053 (9)
C56	0.0239 (11)	0.0257 (12)	0.0444 (15)	0.0025 (9)	0.0100 (10)	0.0056 (10)
C65	0.0215 (10)	0.0208 (10)	0.0375 (13)	0.0014 (8)	0.0068 (9)	−0.0021 (9)
C21	0.0237 (10)	0.0285 (11)	0.0176 (10)	0.0036 (9)	−0.0023 (8)	−0.0008 (8)
C15	0.0478 (15)	0.0165 (11)	0.0321 (13)	0.0019 (10)	−0.0040 (11)	−0.0035 (9)
C66	0.0222 (10)	0.0192 (10)	0.0303 (12)	0.0025 (8)	0.0020 (9)	0.0030 (9)
C37	0.0191 (10)	0.0288 (11)	0.0165 (10)	−0.0007 (8)	0.0044 (8)	0.0014 (8)
C40	0.0208 (10)	0.0246 (11)	0.0281 (11)	−0.0019 (8)	0.0090 (9)	0.0013 (9)
C32	0.0152 (9)	0.0204 (10)	0.0209 (10)	−0.0011 (8)	−0.0006 (7)	0.0008 (8)
C8	0.0242 (10)	0.0288 (11)	0.0168 (10)	−0.0016 (9)	0.0054 (8)	−0.0062 (8)
C36	0.0209 (10)	0.0294 (11)	0.0150 (9)	0.0012 (8)	0.0040 (8)	−0.0021 (8)
C47	0.0176 (10)	0.0285 (11)	0.0282 (11)	−0.0036 (8)	0.0050 (8)	−0.0072 (9)
C9	0.0243 (11)	0.0294 (11)	0.0178 (10)	−0.0046 (9)	0.0076 (8)	−0.0038 (9)
C50	0.0237 (11)	0.0247 (11)	0.0326 (12)	−0.0033 (9)	−0.0001 (9)	0.0003 (9)
C25	0.0182 (9)	0.0164 (9)	0.0204 (10)	0.0010 (7)	0.0000 (7)	0.0021 (8)
C2	0.0187 (10)	0.0361 (13)	0.0243 (11)	−0.0026 (9)	−0.0045 (8)	−0.0018 (9)
C58	0.0237 (11)	0.0341 (13)	0.0415 (15)	0.0107 (10)	0.0029 (10)	−0.0021 (11)
C18	0.0209 (10)	0.0168 (9)	0.0235 (10)	0.0022 (8)	−0.0009 (8)	0.0026 (8)
C54	0.0397 (14)	0.0276 (12)	0.0277 (12)	−0.0073 (10)	0.0048 (10)	0.0000 (10)

B3	0.0166 (10)	0.0184 (11)	0.0226 (11)	0.0001 (8)	0.0018 (8)	0.0023 (9)
C7	0.0247 (11)	0.0254 (11)	0.0251 (11)	0.0040 (9)	0.0051 (9)	−0.0039 (9)
C4	0.0152 (9)	0.0271 (11)	0.0190 (10)	0.0009 (8)	−0.0008 (8)	0.0018 (8)
C20	0.0323 (12)	0.0344 (13)	0.0190 (11)	0.0079 (10)	−0.0030 (9)	0.0050 (9)
C16	0.0530 (16)	0.0161 (10)	0.0316 (13)	0.0048 (10)	−0.0056 (11)	0.0014 (9)
C5	0.0184 (10)	0.0407 (14)	0.0301 (12)	0.0073 (10)	−0.0013 (9)	0.0000 (10)
C35	0.0249 (11)	0.0227 (11)	0.0280 (11)	0.0023 (9)	0.0034 (9)	−0.0069 (9)
C51	0.0299 (13)	0.0297 (13)	0.0423 (15)	−0.0033 (10)	−0.0067 (11)	−0.0048 (11)
C19	0.0408 (14)	0.0243 (11)	0.0269 (12)	0.0065 (10)	−0.0032 (10)	0.0073 (9)
C67	0.0390 (15)	0.0417 (16)	0.0396 (15)	−0.0024 (12)	0.0004 (12)	−0.0041 (12)
C57	0.0216 (12)	0.0357 (14)	0.0593 (18)	0.0044 (10)	0.0125 (12)	0.0048 (13)
C53	0.0624 (19)	0.0363 (14)	0.0243 (13)	−0.0045 (13)	−0.0005 (12)	0.0011 (11)
C33	0.0193 (10)	0.0307 (12)	0.0366 (13)	0.0046 (9)	−0.0032 (9)	−0.0051 (10)
C34	0.0256 (12)	0.0304 (12)	0.0379 (14)	0.0084 (10)	0.0033 (10)	−0.0069 (10)
C52	0.0450 (16)	0.0341 (14)	0.0339 (14)	0.0027 (12)	−0.0131 (12)	−0.0067 (11)
C6	0.0252 (12)	0.0367 (13)	0.0333 (13)	0.0116 (10)	0.0042 (10)	−0.0019 (11)
B2	0.0199 (10)	0.0174 (10)	0.0129 (10)	0.0000 (8)	0.0009 (8)	−0.0008 (8)
B1	0.0203 (11)	0.0172 (10)	0.0181 (10)	−0.0022 (8)	0.0011 (8)	−0.0044 (8)
C68	0.099 (4)	0.053 (2)	0.105 (4)	0.024 (2)	0.044 (3)	0.007 (2)

Geometric parameters (Å, º)

Ce1—O2	2.8099 (14)	C61—B3	1.647 (3)
Ce1—O6	2.8643 (15)	C12—H12	0.9500
Ce1—O3	2.8900 (15)	C62—H62	0.9500
Ce1—O5	2.8808 (15)	C62—C63	1.397 (3)
Ce1—O4	2.8885 (15)	C10—C9	1.403 (3)
Ce1—O1	2.8704 (15)	C41—H41	0.9500
Ce1—N4	2.6383 (17)	C41—C42	1.341 (3)
Ce1—N10	2.6566 (17)	C41—C40	1.430 (3)
Ce1—N12	2.6558 (17)	C29—H29	0.9500
Ce1—N8	2.6458 (17)	C29—C30	1.374 (3)
Ce1—N6	2.6744 (17)	C42—H42	0.9500
Ce1—N2	2.6600 (17)	C45—H45	0.9500
Cl2—C67	1.760 (3)	C45—C46	1.389 (3)
Cl1—C67	1.754 (3)	C63—H63	0.9500
Cl3—C68	1.760 (5)	C63—C64	1.389 (3)
Cl4—C68	1.781 (6)	C30—H30	0.9500
O2—C11	1.380 (2)	C28—H28	0.9500
O2—C14	1.385 (2)	C28—C27	1.346 (3)
O6—C39	1.382 (2)	C46—H46	0.9500
O6—C42	1.379 (3)	C46—C47	1.388 (3)
O3—C21	1.385 (3)	C64—H64	0.9500
O3—C18	1.381 (3)	C64—C65	1.384 (4)
O5—C32	1.378 (3)	C17—C18	1.440 (3)
O5—C35	1.379 (3)	C17—C16	1.400 (3)
O4—C28	1.381 (2)	C3—C2	1.405 (3)
O4—C25	1.379 (3)	C3—C4	1.442 (3)

O1—C7	1.381 (3)	C26—H26	0.9500
O1—C4	1.377 (3)	C26—C27	1.429 (3)
N4—N3	1.363 (2)	C26—C25	1.360 (3)
N4—C10	1.342 (3)	C59—H59	0.9500
N10—N9	1.363 (2)	C59—C58	1.380 (4)
N10—C31	1.343 (3)	C38—C37	1.400 (3)
N12—N11	1.364 (2)	C27—H27	0.9500
N12—C38	1.344 (3)	C56—H56	0.9500
N3—C8	1.349 (3)	C56—C57	1.398 (3)
N3—B1	1.539 (3)	C65—H65	0.9500
N11—C36	1.351 (3)	C65—C66	1.394 (3)
N11—B2	1.539 (3)	C21—H21	0.9500
N7—N8	1.363 (2)	C21—C20	1.341 (3)
N7—C22	1.348 (3)	C15—H15	0.9500
N7—B2	1.532 (3)	C15—C16	1.375 (4)
N1—N2	1.363 (2)	C66—H66	0.9500
N1—C1	1.353 (3)	C37—H37	0.9500
N1—B1	1.539 (3)	C37—C36	1.375 (3)
N8—C24	1.347 (3)	C40—H40	0.9500
N9—C29	1.351 (3)	C32—C33	1.355 (3)
N9—B2	1.540 (3)	C8—H8	0.9500
N6—N5	1.365 (2)	C8—C9	1.378 (3)
N6—C17	1.345 (3)	C36—H36	0.9500
N2—C3	1.343 (3)	C47—H47	0.9500
N5—C15	1.345 (3)	C9—H9	0.9500
N5—B1	1.541 (3)	C50—H50	0.9500
C43—C44	1.405 (3)	C50—C51	1.395 (4)
C43—C48	1.410 (3)	C2—H2	0.9500
C43—B3	1.646 (3)	C58—H58	0.9500
C44—H44	0.9500	C58—C57	1.386 (4)
C44—C45	1.393 (3)	C18—C19	1.355 (3)
C55—C60	1.406 (3)	C54—H54	0.9500
C55—C56	1.400 (3)	C54—C53	1.396 (4)
C55—B3	1.644 (3)	C7—H7	0.9500
C11—C12	1.353 (3)	C7—C6	1.342 (3)
C11—C10	1.442 (3)	C4—C5	1.355 (3)
C60—H60	0.9500	C20—H20	0.9500
C60—C59	1.391 (3)	C20—C19	1.431 (4)
C31—C30	1.403 (3)	C16—H16	0.9500
C31—C32	1.444 (3)	C5—H5	0.9500
C1—H1	0.9500	C5—C6	1.427 (4)
C1—C2	1.372 (3)	C35—H35	0.9500
C14—H14	0.9500	C35—C34	1.343 (3)
C14—C13	1.344 (3)	C51—H51	0.9500
C48—H48	0.9500	C51—C52	1.384 (4)
C48—C47	1.396 (3)	C19—H19	0.9500
C49—C50	1.400 (3)	C67—H67A	0.9900
C49—C54	1.404 (3)	C67—H67B	0.9900

C49—B3	1.650 (3)	C57—H57	0.9500
C13—H13	0.9500	C53—H53	0.9500
C13—C12	1.427 (3)	C53—C52	1.380 (4)
C39—C38	1.445 (3)	C33—H33	0.9500
C39—C40	1.354 (3)	C33—C34	1.430 (4)
C24—C23	1.397 (3)	C34—H34	0.9500
C24—C25	1.437 (3)	C52—H52	0.9500
C23—H23	0.9500	C6—H6	0.9500
C23—C22	1.372 (3)	B2—H2A	1.12 (3)
C22—H22	0.9500	B1—H1A	1.11 (3)
C61—C62	1.403 (3)	C68—H68A	0.9900
C61—C66	1.405 (3)	C68—H68B	0.9900

O2—Ce1—O6	179.40 (5)	N4—C10—C11	119.57 (18)
O2—Ce1—O3	117.47 (4)	N4—C10—C9	111.08 (19)
O2—Ce1—O5	62.00 (5)	C9—C10—C11	129.34 (19)
O2—Ce1—O4	62.69 (4)	C42—C41—H41	126.3
O2—Ce1—O1	118.86 (5)	C42—C41—C40	107.5 (2)
O6—Ce1—O3	61.94 (4)	C40—C41—H41	126.3
O6—Ce1—O5	117.55 (5)	N9—C29—H29	125.6
O6—Ce1—O4	117.91 (5)	N9—C29—C30	108.81 (19)
O6—Ce1—O1	61.59 (5)	C30—C29—H29	125.6
O5—Ce1—O3	62.96 (4)	O6—C42—H42	125.0
O5—Ce1—O4	117.35 (5)	C41—C42—O6	109.9 (2)
O4—Ce1—O3	179.61 (4)	C41—C42—H42	125.0
O1—Ce1—O3	116.56 (5)	C44—C45—H45	119.8
O1—Ce1—O5	178.99 (4)	C46—C45—C44	120.3 (2)
O1—Ce1—O4	63.13 (4)	C46—C45—H45	119.8
N4—Ce1—O2	59.19 (5)	C62—C63—H63	120.0
N4—Ce1—O6	121.09 (5)	C64—C63—C62	120.0 (2)
N4—Ce1—O3	116.79 (5)	C64—C63—H63	120.0
N4—Ce1—O5	64.34 (5)	C31—C30—H30	127.8
N4—Ce1—O4	63.60 (5)	C29—C30—C31	104.35 (18)
N4—Ce1—O1	115.51 (5)	C29—C30—H30	127.8
N4—Ce1—N10	112.47 (5)	O4—C28—H28	125.0
N4—Ce1—N12	179.36 (5)	C27—C28—O4	110.0 (2)
N4—Ce1—N8	112.18 (5)	C27—C28—H28	125.0
N4—Ce1—N6	68.98 (5)	C45—C46—H46	120.7
N4—Ce1—N2	67.61 (5)	C47—C46—C45	118.7 (2)
N10—Ce1—O2	63.98 (5)	C47—C46—H46	120.7
N10—Ce1—O6	115.47 (5)	C63—C64—H64	120.5
N10—Ce1—O3	63.46 (5)	C65—C64—C63	119.0 (2)
N10—Ce1—O5	58.56 (5)	C65—C64—H64	120.5
N10—Ce1—O4	116.46 (5)	N6—C17—C18	120.26 (19)
N10—Ce1—O1	122.16 (5)	N6—C17—C16	110.7 (2)
N10—Ce1—N6	110.58 (5)	C16—C17—C18	129.0 (2)
N10—Ce1—N2	178.97 (5)	N2—C3—C2	110.8 (2)
N12—Ce1—O2	121.44 (5)	N2—C3—C4	119.81 (19)

N12—Ce1—O6	58.28 (5)	C2—C3—C4	129.4 (2)
N12—Ce1—O3	62.97 (5)	C27—C26—H26	126.8
N12—Ce1—O5	115.82 (5)	C25—C26—H26	126.8
N12—Ce1—O4	116.64 (5)	C25—C26—C27	106.4 (2)
N12—Ce1—O1	64.32 (5)	C60—C59—H59	119.8
N12—Ce1—N10	68.00 (5)	C58—C59—C60	120.4 (2)
N12—Ce1—N6	110.49 (5)	C58—C59—H59	119.8
N12—Ce1—N2	111.91 (5)	N12—C38—C39	119.55 (18)
N8—Ce1—O2	65.00 (5)	N12—C38—C37	111.09 (19)
N8—Ce1—O6	115.13 (5)	C37—C38—C39	129.34 (19)
N8—Ce1—O3	121.39 (5)	C28—C27—C26	107.2 (2)
N8—Ce1—O5	117.19 (5)	C28—C27—H27	126.4
N8—Ce1—O4	58.30 (5)	C26—C27—H27	126.4
N8—Ce1—O1	63.81 (5)	C55—C56—H56	118.6
N8—Ce1—N10	69.58 (5)	C57—C56—C55	122.7 (2)
N8—Ce1—N12	68.34 (5)	C57—C56—H56	118.6
N8—Ce1—N6	178.72 (5)	C64—C65—H65	120.0
N8—Ce1—N2	111.38 (5)	C64—C65—C66	120.1 (2)
N6—Ce1—O2	116.24 (5)	C66—C65—H65	120.0
N6—Ce1—O6	63.62 (5)	O3—C21—H21	124.9
N6—Ce1—O3	57.96 (5)	C20—C21—O3	110.3 (2)
N6—Ce1—O5	63.68 (5)	C20—C21—H21	124.9
N6—Ce1—O4	122.34 (5)	N5—C15—H15	125.6
N6—Ce1—O1	115.32 (5)	N5—C15—C16	108.7 (2)
N2—Ce1—O2	116.67 (5)	C16—C15—H15	125.6
N2—Ce1—O6	63.88 (5)	C61—C66—H66	118.5
N2—Ce1—O3	115.55 (5)	C65—C66—C61	123.0 (2)
N2—Ce1—O5	120.88 (5)	C65—C66—H66	118.5
N2—Ce1—O4	64.53 (5)	C38—C37—H37	127.8
N2—Ce1—O1	58.38 (5)	C36—C37—C38	104.30 (19)
N2—Ce1—N6	68.45 (5)	C36—C37—H37	127.8
C11—O2—Ce1	120.06 (12)	C39—C40—C41	106.3 (2)
C11—O2—C14	106.01 (16)	C39—C40—H40	126.9
C14—O2—Ce1	133.48 (12)	C41—C40—H40	126.9
C39—O6—Ce1	120.14 (12)	O5—C32—C31	115.53 (18)
C42—O6—Ce1	133.27 (13)	C33—C32—O5	110.1 (2)
C42—O6—C39	106.43 (17)	C33—C32—C31	134.4 (2)
C21—O3—Ce1	133.67 (13)	N3—C8—H8	125.5
C18—O3—Ce1	120.11 (12)	N3—C8—C9	108.91 (19)
C18—O3—C21	106.17 (17)	C9—C8—H8	125.5
C32—O5—Ce1	119.16 (12)	N11—C36—C37	108.83 (19)
C32—O5—C35	106.35 (17)	N11—C36—H36	125.6
C35—O5—Ce1	134.48 (13)	C37—C36—H36	125.6
C28—O4—Ce1	134.24 (13)	C48—C47—H47	119.8
C25—O4—Ce1	118.88 (12)	C46—C47—C48	120.4 (2)
C25—O4—C28	106.53 (17)	C46—C47—H47	119.8
C7—O1—Ce1	133.57 (14)	C10—C9—H9	128.0
C4—O1—Ce1	119.71 (12)	C8—C9—C10	104.08 (19)

C4—O1—C7	106.41 (17)	C8—C9—H9	128.0
N3—N4—Ce1	128.49 (12)	C49—C50—H50	118.6
C10—N4—Ce1	125.63 (13)	C51—C50—C49	122.8 (2)
C10—N4—N3	105.87 (16)	C51—C50—H50	118.6
N9—N10—Ce1	127.22 (12)	O4—C25—C24	115.42 (18)
C31—N10—Ce1	126.11 (13)	C26—C25—O4	109.83 (19)
C31—N10—N9	105.88 (16)	C26—C25—C24	134.7 (2)
N11—N12—Ce1	127.33 (12)	C1—C2—C3	104.4 (2)
C38—N12—Ce1	126.94 (13)	C1—C2—H2	127.8
C38—N12—N11	105.72 (16)	C3—C2—H2	127.8
N4—N3—B1	121.33 (16)	C59—C58—H58	120.5
C8—N3—N4	110.06 (17)	C59—C58—C57	118.9 (2)
C8—N3—B1	128.61 (18)	C57—C58—H58	120.5
N12—N11—B2	121.56 (16)	O3—C18—C17	114.86 (18)
C36—N11—N12	110.05 (17)	C19—C18—O3	109.9 (2)
C36—N11—B2	128.33 (18)	C19—C18—C17	135.2 (2)
N8—N7—B2	121.53 (16)	C49—C54—H54	118.5
C22—N7—N8	110.18 (17)	C53—C54—C49	123.1 (2)
C22—N7—B2	128.23 (18)	C53—C54—H54	118.5
N2—N1—B1	121.68 (17)	C43—B3—C49	112.47 (18)
C1—N1—N2	110.06 (18)	C43—B3—C61	104.84 (17)
C1—N1—B1	128.23 (19)	C55—B3—C43	111.94 (18)
N7—N8—Ce1	127.71 (12)	C55—B3—C49	103.99 (17)
C24—N8—Ce1	126.69 (13)	C55—B3—C61	112.87 (18)
C24—N8—N7	105.40 (16)	C61—B3—C49	110.96 (17)
N10—N9—B2	121.41 (16)	O1—C7—H7	125.0
C29—N9—N10	110.05 (17)	C6—C7—O1	110.1 (2)
C29—N9—B2	128.52 (18)	C6—C7—H7	125.0
N5—N6—Ce1	127.54 (13)	O1—C4—C3	115.33 (18)
C17—N6—Ce1	126.43 (14)	C5—C4—O1	109.8 (2)
C17—N6—N5	105.69 (17)	C5—C4—C3	134.8 (2)
N1—N2—Ce1	127.58 (13)	C21—C20—H20	126.5
C3—N2—Ce1	126.47 (14)	C21—C20—C19	107.0 (2)
C3—N2—N1	105.88 (17)	C19—C20—H20	126.5
N6—N5—B1	121.18 (17)	C17—C16—H16	127.7
C15—N5—N6	110.30 (19)	C15—C16—C17	104.6 (2)
C15—N5—B1	128.50 (19)	C15—C16—H16	127.7
C44—C43—C48	114.9 (2)	C4—C5—H5	126.7
C44—C43—B3	123.24 (19)	C4—C5—C6	106.6 (2)
C48—C43—B3	121.62 (19)	C6—C5—H5	126.7
C43—C44—H44	118.5	O5—C35—H35	125.0
C45—C44—C43	123.0 (2)	C34—C35—O5	110.1 (2)
C45—C44—H44	118.5	C34—C35—H35	125.0
C60—C55—B3	120.9 (2)	C50—C51—H51	119.9
C56—C55—C60	115.1 (2)	C52—C51—C50	120.3 (2)
C56—C55—B3	123.8 (2)	C52—C51—H51	119.9
O2—C11—C10	115.14 (17)	C18—C19—C20	106.7 (2)
C12—C11—O2	110.13 (18)	C18—C19—H19	126.7

C12—C11—C10	134.73 (19)	C20—C19—H19	126.7
C55—C60—H60	118.6	Cl2—C67—H67A	109.6
C59—C60—C55	122.7 (2)	Cl2—C67—H67B	109.6
C59—C60—H60	118.6	Cl1—C67—Cl2	110.35 (17)
N10—C31—C30	110.92 (19)	Cl1—C67—H67A	109.6
N10—C31—C32	120.07 (18)	Cl1—C67—H67B	109.6
C30—C31—C32	129.02 (19)	H67A—C67—H67B	108.1
N1—C1—H1	125.6	C56—C57—H57	120.0
N1—C1—C2	108.8 (2)	C58—C57—C56	120.1 (2)
C2—C1—H1	125.6	C58—C57—H57	120.0
O2—C14—H14	124.9	C54—C53—H53	120.0
C13—C14—O2	110.19 (19)	C52—C53—C54	119.9 (3)
C13—C14—H14	124.9	C52—C53—H53	120.0
C43—C48—H48	118.7	C32—C33—H33	126.8
C47—C48—C43	122.7 (2)	C32—C33—C34	106.3 (2)
C47—C48—H48	118.7	C34—C33—H33	126.8
C50—C49—C54	114.9 (2)	C35—C34—C33	107.2 (2)
C50—C49—B3	122.2 (2)	C35—C34—H34	126.4
C54—C49—B3	122.7 (2)	C33—C34—H34	126.4
C14—C13—H13	126.5	C51—C52—H52	120.5
C14—C13—C12	107.03 (19)	C53—C52—C51	119.0 (3)
C12—C13—H13	126.5	C53—C52—H52	120.5
O6—C39—C38	115.01 (17)	C7—C6—C5	107.1 (2)
C40—C39—O6	109.90 (19)	C7—C6—H6	126.4
C40—C39—C38	135.1 (2)	C5—C6—H6	126.4
N8—C24—C23	111.21 (19)	N11—B2—N9	109.63 (17)
N8—C24—C25	120.01 (18)	N11—B2—H2A	108.2 (14)
C23—C24—C25	128.8 (2)	N7—B2—N11	108.75 (17)
C24—C23—H23	127.9	N7—B2—N9	109.29 (16)
C22—C23—C24	104.26 (19)	N7—B2—H2A	110.1 (14)
C22—C23—H23	127.9	N9—B2—H2A	110.8 (14)
N7—C22—C23	108.95 (19)	N3—B1—N1	109.33 (17)
N7—C22—H22	125.5	N3—B1—N5	108.46 (17)
C23—C22—H22	125.5	N3—B1—H1A	110.6 (14)
C62—C61—C66	115.0 (2)	N1—B1—N5	109.62 (17)
C62—C61—B3	124.55 (19)	N1—B1—H1A	109.7 (14)
C66—C61—B3	120.2 (2)	N5—B1—H1A	109.1 (14)
C11—C12—C13	106.63 (19)	Cl3—C68—Cl4	112.1 (3)
C11—C12—H12	126.7	Cl3—C68—H68A	109.2
C13—C12—H12	126.7	Cl3—C68—H68B	109.2
C61—C62—H62	118.6	Cl4—C68—H68A	109.2
C63—C62—C61	122.8 (2)	Cl4—C68—H68B	109.2
C63—C62—H62	118.6	H68A—C68—H68B	107.9
Ce1—O2—C11—C12	−172.83 (14)	C1—N1—B1—N3	−121.5 (2)
Ce1—O2—C11—C10	7.6 (2)	C1—N1—B1—N5	119.7 (2)
Ce1—O2—C14—C13	172.08 (14)	C14—O2—C11—C12	0.4 (2)
Ce1—O6—C39—C38	−3.4 (2)	C14—O2—C11—C10	−179.16 (17)

Ce1—O6—C39—C40	175.87 (14)	C14—C13—C12—C11	0.8 (3)
Ce1—O6—C42—C41	−175.38 (15)	C48—C43—C44—C45	−1.0 (3)
Ce1—O3—C21—C20	−177.36 (15)	C48—C43—B3—C55	45.5 (3)
Ce1—O3—C18—C17	−0.8 (2)	C48—C43—B3—C49	162.13 (19)
Ce1—O3—C18—C19	178.11 (16)	C48—C43—B3—C61	−77.2 (2)
Ce1—O5—C32—C31	1.7 (2)	C49—C50—C51—C52	−0.2 (4)
Ce1—O5—C32—C33	−178.97 (16)	C49—C54—C53—C52	0.9 (5)
Ce1—O5—C35—C34	178.95 (16)	C39—O6—C42—C41	−0.2 (3)
Ce1—O4—C28—C27	−172.82 (14)	C39—C38—C37—C36	−178.3 (2)
Ce1—O4—C25—C24	−7.5 (2)	C24—C23—C22—N7	0.5 (3)
Ce1—O4—C25—C26	173.67 (14)	C23—C24—C25—O4	−177.7 (2)
Ce1—O1—C7—C6	−173.24 (16)	C23—C24—C25—C26	0.7 (4)
Ce1—O1—C4—C3	−6.2 (2)	C22—N7—N8—Ce1	174.74 (14)
Ce1—O1—C4—C5	174.40 (16)	C22—N7—N8—C24	−0.4 (2)
Ce1—N4—N3—C8	178.46 (14)	C22—N7—B2—N11	−115.3 (2)
Ce1—N4—N3—B1	−1.5 (3)	C22—N7—B2—N9	125.1 (2)
Ce1—N4—C10—C11	1.4 (3)	C61—C62—C63—C64	0.6 (3)
Ce1—N4—C10—C9	−178.74 (14)	C12—C11—C10—N4	174.5 (2)
Ce1—N10—N9—C29	169.61 (13)	C12—C11—C10—C9	−5.3 (4)
Ce1—N10—N9—B2	−8.8 (2)	C62—C61—C66—C65	−0.8 (3)
Ce1—N10—C31—C30	−169.78 (13)	C62—C61—B3—C43	102.4 (2)
Ce1—N10—C31—C32	9.8 (3)	C62—C61—B3—C55	−19.7 (3)
Ce1—N12—N11—C36	179.60 (14)	C62—C61—B3—C49	−136.0 (2)
Ce1—N12—N11—B2	−3.0 (3)	C62—C63—C64—C65	−0.9 (3)
Ce1—N12—C38—C39	−0.8 (3)	C10—N4—N3—C8	−0.3 (2)
Ce1—N12—C38—C37	−179.49 (14)	C10—N4—N3—B1	179.77 (18)
Ce1—N8—C24—C23	−174.50 (14)	C10—C11—C12—C13	178.7 (2)
Ce1—N8—C24—C25	5.9 (3)	C29—N9—B2—N11	127.5 (2)
Ce1—N6—N5—C15	−173.11 (16)	C29—N9—B2—N7	−113.4 (2)
Ce1—N6—N5—B1	5.3 (3)	C42—O6—C39—C38	−179.34 (18)
Ce1—N6—C17—C18	−8.0 (3)	C42—O6—C39—C40	−0.1 (2)
Ce1—N6—C17—C16	173.16 (17)	C42—C41—C40—C39	−0.4 (3)
Ce1—N2—C3—C2	177.50 (15)	C45—C46—C47—C48	−0.3 (3)
Ce1—N2—C3—C4	−2.6 (3)	C63—C64—C65—C66	0.4 (3)
O2—C11—C12—C13	−0.8 (2)	C30—C31—C32—O5	172.5 (2)
O2—C11—C10—N4	−6.0 (3)	C30—C31—C32—C33	−6.7 (4)
O2—C11—C10—C9	174.2 (2)	C28—O4—C25—C24	178.30 (18)
O2—C14—C13—C12	−0.6 (3)	C28—O4—C25—C26	−0.5 (2)
O6—C39—C38—N12	2.8 (3)	C64—C65—C66—C61	0.5 (4)
O6—C39—C38—C37	−178.8 (2)	C17—N6—N5—C15	0.6 (3)
O6—C39—C40—C41	0.3 (3)	C17—N6—N5—B1	178.97 (19)
O3—C21—C20—C19	−0.4 (3)	C17—C18—C19—C20	178.1 (3)
O3—C18—C19—C20	−0.4 (3)	C3—C4—C5—C6	−179.2 (3)
O5—C32—C33—C34	−0.4 (3)	C59—C58—C57—C56	−0.2 (5)
O5—C35—C34—C33	0.2 (3)	C38—N12—N11—C36	0.6 (2)
O4—C28—C27—C26	0.4 (3)	C38—N12—N11—B2	178.08 (18)
O1—C7—C6—C5	−0.1 (3)	C38—C39—C40—C41	179.3 (2)
O1—C4—C5—C6	0.0 (3)	C38—C37—C36—N11	0.2 (2)

N4—N3—C8—C9	0.4 (3)	C27—C26—C25—O4	0.7 (3)
N4—N3—B1—N1	−58.3 (2)	C27—C26—C25—C24	−177.7 (2)
N4—N3—B1—N5	61.2 (2)	C56—C55—C60—C59	−0.3 (3)
N4—C10—C9—C8	0.2 (3)	C56—C55—B3—C43	20.9 (3)
N10—N9—C29—C30	0.4 (2)	C56—C55—B3—C49	−100.8 (3)
N10—N9—B2—N11	−54.5 (2)	C56—C55—B3—C61	138.9 (2)
N10—N9—B2—N7	64.6 (2)	C21—O3—C18—C17	−178.72 (19)
N10—C31—C30—C29	−0.3 (2)	C21—O3—C18—C19	0.2 (3)
N10—C31—C32—O5	−7.0 (3)	C21—C20—C19—C18	0.5 (3)
N10—C31—C32—C33	173.8 (3)	C15—N5—B1—N3	115.2 (3)
N12—N11—C36—C37	−0.5 (2)	C15—N5—B1—N1	−125.5 (2)
N12—N11—B2—N7	−58.2 (2)	C66—C61—C62—C63	0.3 (3)
N12—N11—B2—N9	61.2 (2)	C66—C61—B3—C43	−72.1 (2)
N12—C38—C37—C36	0.2 (2)	C66—C61—B3—C55	165.8 (2)
N3—N4—C10—C11	−179.84 (18)	C66—C61—B3—C49	49.6 (3)
N3—N4—C10—C9	0.0 (2)	C40—C39—C38—N12	−176.2 (2)
N3—C8—C9—C10	−0.3 (3)	C40—C39—C38—C37	2.2 (4)
N11—N12—C38—C39	178.13 (18)	C40—C41—C42—O6	0.4 (3)
N11—N12—C38—C37	−0.5 (2)	C32—O5—C35—C34	−0.4 (3)
N7—N8—C24—C23	0.7 (2)	C32—C31—C30—C29	−179.8 (2)
N7—N8—C24—C25	−178.97 (18)	C32—C33—C34—C35	0.2 (3)
N1—N2—C3—C2	0.2 (2)	C8—N3—B1—N1	121.7 (2)
N1—N2—C3—C4	−179.93 (19)	C8—N3—B1—N5	−118.8 (2)
N1—C1—C2—C3	0.3 (3)	C36—N11—B2—N7	118.7 (2)
N8—N7—C22—C23	−0.1 (3)	C36—N11—B2—N9	−121.8 (2)
N8—N7—B2—N11	61.5 (2)	C50—C49—C54—C53	−1.5 (4)
N8—N7—B2—N9	−58.1 (2)	C50—C49—B3—C43	145.8 (2)
N8—C24—C23—C22	−0.7 (3)	C50—C49—B3—C55	−92.9 (2)
N8—C24—C25—O4	1.8 (3)	C50—C49—B3—C61	28.7 (3)
N8—C24—C25—C26	−179.8 (2)	C50—C51—C52—C53	−0.5 (4)
N9—N10—C31—C30	0.5 (2)	C25—O4—C28—C27	0.0 (2)
N9—N10—C31—C32	−179.90 (18)	C25—C24—C23—C22	178.9 (2)
N9—C29—C30—C31	−0.1 (2)	C25—C26—C27—C28	−0.7 (3)
N6—N5—C15—C16	−0.3 (3)	C2—C3—C4—O1	−174.3 (2)
N6—N5—B1—N3	−62.9 (2)	C2—C3—C4—C5	4.9 (4)
N6—N5—B1—N1	56.4 (2)	C18—O3—C21—C20	0.2 (3)
N6—C17—C18—O3	5.3 (3)	C18—C17—C16—C15	−178.3 (2)
N6—C17—C18—C19	−173.2 (3)	C54—C49—C50—C51	1.1 (4)
N6—C17—C16—C15	0.4 (3)	C54—C49—B3—C43	−40.0 (3)
N2—N1—C1—C2	−0.2 (3)	C54—C49—B3—C55	81.3 (3)
N2—N1—B1—N3	56.3 (2)	C54—C49—B3—C61	−157.1 (2)
N2—N1—B1—N5	−62.5 (2)	C54—C53—C52—C51	0.2 (5)
N2—C3—C2—C1	−0.3 (3)	B3—C43—C44—C45	−176.0 (2)
N2—C3—C4—O1	5.9 (3)	B3—C43—C48—C47	177.1 (2)
N2—C3—C4—C5	−175.0 (3)	B3—C55—C60—C59	−175.2 (2)
N5—N6—C17—C18	178.24 (19)	B3—C55—C56—C57	175.5 (3)
N5—N6—C17—C16	−0.6 (3)	B3—C49—C50—C51	175.7 (2)
N5—C15—C16—C17	−0.1 (3)	B3—C49—C54—C53	−176.1 (3)

C43—C44—C45—C46	−0.5 (3)	B3—C61—C62—C63	−174.4 (2)
C43—C48—C47—C46	−1.4 (3)	B3—C61—C66—C65	174.1 (2)
C44—C43—C48—C47	1.9 (3)	C7—O1—C4—C3	179.36 (19)
C44—C43—B3—C55	−139.8 (2)	C7—O1—C4—C5	0.0 (3)
C44—C43—B3—C49	−23.1 (3)	C4—O1—C7—C6	0.0 (3)
C44—C43—B3—C61	97.5 (2)	C4—C3—C2—C1	179.8 (2)
C44—C45—C46—C47	1.2 (3)	C4—C5—C6—C7	0.1 (3)
C55—C60—C59—C58	−0.4 (4)	C16—C17—C18—O3	−176.1 (2)
C55—C56—C57—C58	−0.6 (5)	C16—C17—C18—C19	5.4 (5)
C11—O2—C14—C13	0.1 (2)	C35—O5—C32—C31	−178.86 (19)
C11—C10—C9—C8	−180.0 (2)	C35—O5—C32—C33	0.5 (3)
C60—C55—C56—C57	0.8 (4)	B2—N11—C36—C37	−177.7 (2)
C60—C55—B3—C43	−164.8 (2)	B2—N7—N8—Ce1	−2.6 (3)
C60—C55—B3—C49	73.6 (2)	B2—N7—N8—C24	−177.68 (18)
C60—C55—B3—C61	−46.8 (3)	B2—N7—C22—C23	177.0 (2)
C60—C59—C58—C57	0.6 (4)	B2—N9—C29—C30	178.61 (19)
C31—N10—N9—C29	−0.6 (2)	B1—N3—C8—C9	−179.6 (2)
C31—N10—N9—B2	−178.93 (17)	B1—N1—N2—Ce1	4.6 (3)
C31—C32—C33—C34	178.8 (2)	B1—N1—N2—C3	−178.16 (18)
C1—N1—N2—Ce1	−177.23 (14)	B1—N1—C1—C2	177.8 (2)
C1—N1—N2—C3	0.0 (2)	B1—N5—C15—C16	−178.6 (2)

Bis{hydrotris[3-(2-furyl)pyrazol-1-yl]borato}dysprosium(III) tetraphenylborate dichloromethane monosolvate (1Dy)

Crystal data

$[Dy(C_{21}H_{16}BN_6O_3)_2](C_{24}H_{20}B)\cdot 2CH_2Cl_2$
M_r = 1389.05
Triclinic, $P\overline{1}$
a = 12.1461 (7) Å
b = 16.1883 (8) Å
c = 17.1795 (10) Å
α = 102.659 (2)°
β = 103.322 (2)°
γ = 95.948 (2)°
V = 3164.6 (3) Å^3

Z = 2
$F(000)$ = 1406
D_x = 1.458 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9633 reflections
θ = 2.5–29.8°
μ = 1.33 mm^{-1}
T = 100 K
Plate, clear colourless
0.3 × 0.2 × 0.05 mm

Data collection

Bruker D8 QUEST diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.610, T_{max} = 0.747
245023 measured reflections

12926 independent reflections
11705 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 26.4°, θ_{min} = 2.3°
h = −15→15
k = −20→20
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.105

S = 1.08
12926 reflections
930 parameters
14 restraints

Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0233P)^2 + 13.8441P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 2.71$ e Å^{-3}
$\Delta\rho_{min} = -1.74$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data were collected on a Bruker D8 QUEST diffractometer at 100 K, fitted with a CCD area detector employing a mirror-monochromatic Mo *Kα* radiation source (λ = 0.71073 Å). Integration and scaling data of collections were analysed using *APEX3* software. All data was collected with exposures times of 10 s with 1° frame sweeps on ω and φ scans. Multi-scan absorption corrections were used for all compounds. Data was solved in *APEX3* software by intrinsic phasing methods using *SHELXL2019* (Sheldrick, 2015*b*). Refinement of the crystal data was carried out using least-squares refinement methods employed by *SHELXT* (Sheldrick, 2015*a*), with all non-H atoms having anisotropic displacement parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Dy1	0.81975 (2)	0.19655 (2)	0.76273 (2)	0.02868 (6)	
O3	0.8374 (2)	0.35415 (17)	0.86982 (18)	0.0334 (6)	
O1	1.0496 (2)	0.15674 (17)	0.71406 (17)	0.0300 (6)	
O5	0.6197 (2)	0.23463 (17)	0.80402 (16)	0.0282 (6)	
O4	0.8071 (3)	0.01609 (18)	0.64945 (17)	0.0348 (6)	
O2	0.6104 (2)	0.1262 (2)	0.63446 (17)	0.0389 (7)	
O6	1.0413 (2)	0.26403 (18)	0.89264 (19)	0.0371 (7)	
N2	0.9462 (3)	0.08824 (19)	0.81638 (18)	0.0260 (6)	
N8	0.8362 (3)	0.1709 (2)	0.6129 (2)	0.0290 (7)	
N5	0.8188 (3)	0.1408 (2)	0.9496 (2)	0.0328 (7)	
N7	0.8431 (3)	0.2345 (3)	0.5724 (2)	0.0395 (9)	
N1	0.9180 (3)	0.0415 (2)	0.8682 (2)	0.0300 (7)	
C61	0.2508 (3)	0.68589 (19)	0.6992 (2)	0.0264 (8)	
C66	0.3022 (3)	0.7680 (2)	0.7461 (3)	0.0245 (14)	0.5
H66	0.383211	0.781132	0.766883	0.029*	0.5
C65	0.2351 (5)	0.8308 (2)	0.7625 (4)	0.0290 (16)	0.5
H65	0.270199	0.886946	0.794558	0.035*	0.5
C64	0.1165 (4)	0.8116 (3)	0.7320 (4)	0.032 (3)	0.5
H64	0.070654	0.854561	0.743267	0.038*	0.5
C63	0.0651 (3)	0.7295 (4)	0.6851 (4)	0.0275 (19)	0.5
H63	−0.015881	0.716361	0.664300	0.033*	0.5
C62	0.1323 (3)	0.6667 (2)	0.6687 (3)	0.0265 (19)	0.5
H62	0.097130	0.610546	0.636623	0.032*	0.5
C7	1.1205 (4)	0.1852 (3)	0.6694 (2)	0.0328 (9)	
H7	1.102090	0.222299	0.634152	0.039*	
N10	0.7141 (3)	0.3006 (2)	0.7015 (2)	0.0298 (7)	
C55	0.4364 (3)	0.6493 (2)	0.6412 (2)	0.0268 (8)	
C54	0.2887 (3)	0.4436 (2)	0.6434 (2)	0.0268 (8)	

H54	0.341533	0.443557	0.693685	0.032*
C21	0.8482 (4)	0.4373 (2)	0.8610 (3)	0.0418 (11)
H21	0.847362	0.452886	0.810723	0.050*
C43	0.4039 (3)	0.6028 (2)	0.7769 (2)	0.0251 (7)
C4	1.1073 (3)	0.1046 (2)	0.7552 (2)	0.0265 (7)
N12	0.9684 (3)	0.3148 (2)	0.7527 (2)	0.0321 (7)
C23	0.8538 (4)	0.1158 (4)	0.4839 (3)	0.0472 (12)
H23	0.860017	0.076352	0.435905	0.057*
N6	0.8233 (3)	0.2067 (2)	0.91210 (19)	0.0267 (6)
N4	0.6856 (3)	0.0692 (2)	0.7693 (2)	0.0287 (7)
C2	1.0867 (3)	0.0099 (3)	0.8526 (2)	0.0317 (8)
H2	1.155915	−0.013342	0.857014	0.038*
C18	0.8436 (3)	0.3600 (3)	0.9521 (3)	0.0352 (9)
C25	0.8423 (3)	0.0179 (3)	0.5804 (2)	0.0296 (8)
N3	0.7030 (3)	0.0253 (2)	0.8297 (2)	0.0339 (8)
C49	0.2701 (3)	0.5217 (2)	0.6263 (2)	0.0226 (7)
C22	0.8534 (4)	0.2018 (4)	0.4955 (3)	0.0537 (14)
H22	0.859343	0.233555	0.455869	0.064*
C3	1.0481 (3)	0.0678 (2)	0.8063 (2)	0.0261 (7)
C44	0.3520 (4)	0.6121 (3)	0.8424 (2)	0.0349 (9)
H44	0.279602	0.630842	0.835546	0.042*
C26	0.8722 (4)	−0.0582 (3)	0.5495 (3)	0.0424 (11)
H26	0.899524	−0.073079	0.501599	0.051*
C35	0.5595 (4)	0.2110 (3)	0.8569 (2)	0.0317 (8)
H35	0.577589	0.170054	0.887900	0.038*
C6	1.2169 (4)	0.1537 (3)	0.6824 (3)	0.0402 (10)
H6	1.279132	0.164647	0.659302	0.048*
C24	0.8430 (3)	0.0984 (3)	0.5582 (2)	0.0331 (9)
N9	0.7413 (3)	0.3407 (3)	0.6448 (3)	0.0462 (10)
C17	0.8360 (3)	0.2787 (3)	0.9724 (2)	0.0332 (9)
C32	0.5651 (3)	0.2942 (3)	0.7716 (2)	0.0320 (8)
C5	1.2109 (4)	0.1002 (3)	0.7373 (3)	0.0373 (9)
H5	1.267245	0.068112	0.757463	0.045*
C16	0.8402 (4)	0.2588 (3)	1.0483 (3)	0.0478 (12)
H16	0.849067	0.297574	1.100385	0.057*
C53	0.2331 (4)	0.3652 (2)	0.5897 (3)	0.0373 (10)
H53	0.250484	0.313233	0.602888	0.045*
N11	0.9533 (3)	0.3555 (2)	0.6897 (3)	0.0416 (9)
C28	0.8164 (4)	−0.0635 (3)	0.6623 (3)	0.0467 (11)
H28	0.798448	−0.082520	0.707143	0.056*
C27	0.8548 (4)	−0.1114 (3)	0.6025 (3)	0.0481 (12)
H27	0.867599	−0.169085	0.596948	0.058*
C15	0.8289 (4)	0.1717 (4)	1.0308 (3)	0.0476 (12)
H15	0.828168	0.138052	1.069670	0.057*
C46	0.5067 (4)	0.5676 (3)	0.9293 (3)	0.0534 (14)
H46	0.541048	0.555352	0.980177	0.064*
C1	1.0007 (4)	−0.0050 (3)	0.8899 (3)	0.0370 (9)
H1	0.999614	−0.042214	0.925546	0.044*

C52	0.1531 (4)	0.3626 (3)	0.5176 (3)	0.0415 (11)	
H52	0.112704	0.309293	0.482035	0.050*	
C31	0.6164 (4)	0.3258 (3)	0.7140 (3)	0.0359 (9)	
C45	0.4028 (4)	0.5950 (3)	0.9175 (3)	0.0490 (13)	
H45	0.364915	0.602377	0.960538	0.059*	
C58	0.6077 (4)	0.7059 (3)	0.5673 (4)	0.0530 (13)	
H58A	0.674412	0.727502	0.553460	0.064*	0.5
H58	0.653849	0.727037	0.535921	0.064*	0.5
C48	0.5103 (4)	0.5760 (3)	0.7926 (3)	0.0375 (9)	
H48	0.550209	0.569613	0.750661	0.045*	
C51	0.1326 (4)	0.4385 (3)	0.4979 (3)	0.0442 (11)	
H51	0.078918	0.437851	0.447753	0.053*	
C20	0.8598 (4)	0.4922 (3)	0.9338 (4)	0.0514 (13)	
H20	0.868405	0.552919	0.944294	0.062*	
C50	0.1907 (4)	0.5162 (3)	0.5515 (3)	0.0373 (9)	
H50	0.175584	0.567886	0.536546	0.045*	
C39	1.1154 (3)	0.3225 (3)	0.8751 (3)	0.0387 (10)	
C34	0.4720 (4)	0.2543 (3)	0.8578 (3)	0.0400 (10)	
H34	0.417714	0.249991	0.889288	0.048*	
C14	0.5529 (4)	0.1482 (4)	0.5650 (3)	0.0493 (12)	
H14	0.583151	0.189452	0.540392	0.059*	
C38	1.0708 (4)	0.3523 (3)	0.8036 (3)	0.0384 (10)	
C19	0.8569 (4)	0.4432 (3)	0.9925 (3)	0.0478 (12)	
H19	0.863218	0.465032	1.049698	0.057*	
B3	0.3397 (3)	0.6157 (2)	0.6859 (2)	0.0221 (8)	
C37	1.1204 (5)	0.4166 (3)	0.7744 (4)	0.0569 (16)	
H37	1.192379	0.452873	0.799363	0.068*	
C42	1.0990 (4)	0.2434 (3)	0.9620 (3)	0.0450 (11)	
H42	1.068422	0.203896	0.988152	0.054*	
C56A	0.5003 (8)	0.5909 (7)	0.6003 (6)	0.023 (2)	0.5
H56A	0.484499	0.532093	0.600002	0.028*	0.5
C33	0.4750 (4)	0.3084 (3)	0.8028 (3)	0.0423 (11)	
H33	0.423521	0.346988	0.790663	0.051*	
C47	0.5606 (4)	0.5581 (3)	0.8668 (3)	0.0500 (12)	
H47	0.632860	0.539223	0.874436	0.060*	
C11	0.5359 (3)	0.0643 (3)	0.6486 (3)	0.0383 (10)	
C9	0.5323 (4)	−0.0317 (3)	0.7483 (3)	0.0453 (12)	
H9	0.458881	−0.066294	0.724843	0.054*	
C12	0.4361 (4)	0.0486 (4)	0.5904 (3)	0.0530 (13)	
H12	0.370508	0.008654	0.586084	0.064*	
C8	0.6115 (4)	−0.0352 (3)	0.8168 (3)	0.0432 (11)	
H8	0.603711	−0.073935	0.850223	0.052*	
C40	1.2171 (4)	0.3391 (4)	0.9319 (3)	0.0573 (15)	
H40	1.283040	0.377451	0.934052	0.069*	
C13	0.4461 (4)	0.1015 (4)	0.5373 (3)	0.0594 (16)	
H13	0.388589	0.104152	0.490308	0.071*	
C41	1.2065 (4)	0.2881 (4)	0.9877 (3)	0.0592 (15)	
H41	1.264387	0.285798	1.034593	0.071*	

C30	0.5802 (5)	0.3818 (4)	0.6662 (4)	0.0634 (18)	
H30	0.514126	0.408863	0.663744	0.076*	
C29	0.6618 (6)	0.3891 (4)	0.6232 (4)	0.074 (2)	
H29	0.661954	0.422960	0.584530	0.088*	
C10	0.5816 (3)	0.0337 (3)	0.7193 (3)	0.0357 (9)	
C57A	0.5822 (10)	0.6141 (8)	0.5619 (8)	0.026 (2)	0.5
H57A	0.619728	0.573229	0.533815	0.032*	0.5
B1	0.8109 (4)	0.0483 (3)	0.9011 (3)	0.0340 (10)	
C36	1.0442 (5)	0.4168 (3)	0.7024 (4)	0.0551 (15)	
H36	1.053523	0.453557	0.667446	0.066*	
C59A	0.5405 (6)	0.7584 (5)	0.5906 (4)	0.0244 (14)	0.5
H59A	0.548486	0.814723	0.582536	0.029*	0.5
B2	0.8496 (5)	0.3292 (4)	0.6150 (4)	0.0477 (14)	
C60A	0.4569 (6)	0.7319 (4)	0.6275 (4)	0.0213 (13)	0.5
Cl2	0.8093 (5)	0.8025 (4)	0.8276 (5)	0.0776 (18)	0.5
Cl1	0.8010 (3)	0.61762 (19)	0.7731 (2)	0.0680 (8)	0.5
C67	0.7307 (12)	0.7068 (7)	0.7639 (9)	0.069 (4)	0.5
H67A	0.715016	0.710964	0.705841	0.083*	0.5
H67B	0.656160	0.697174	0.777271	0.083*	0.5
H1A	0.810 (4)	0.004 (3)	0.940 (3)	0.037 (12)*	
H2A	0.856 (4)	0.372 (3)	0.572 (3)	0.043 (13)*	
C60	0.5116 (8)	0.7291 (6)	0.6866 (6)	0.046 (2)	0.5
H60	0.503006	0.759683	0.738205	0.055*	0.5
C59	0.5972 (10)	0.7605 (7)	0.6533 (7)	0.056 (3)	0.5
H59	0.647566	0.812888	0.681257	0.068*	0.5
C57	0.5524 (13)	0.6362 (9)	0.5458 (9)	0.042 (3)	0.5
H57	0.570684	0.596546	0.502925	0.050*	0.5
C56	0.4621 (11)	0.6055 (7)	0.5770 (7)	0.036 (2)	0.5
H56	0.418585	0.550280	0.549540	0.044*	0.5
C66A	0.2622 (9)	0.7686 (6)	0.6920 (6)	0.043 (2)	0.5
H66A	0.327869	0.790680	0.677165	0.052*	0.5
H60A	0.411 (9)	0.775 (7)	0.652 (6)	0.052*	0.5
C62A	0.1418 (8)	0.6583 (7)	0.7082 (7)	0.045 (3)	0.5
H62A	0.121 (9)	0.608 (7)	0.702 (7)	0.054*	0.5
C65A	0.1804 (13)	0.8232 (7)	0.7057 (7)	0.058 (3)	0.5
H65A	0.197220	0.881335	0.704040	0.069*	0.5
C63A	0.0612 (10)	0.7125 (10)	0.7211 (7)	0.062 (4)	0.5
H63A	−0.008684	0.689903	0.730279	0.074*	0.5
C64A	0.0812 (18)	0.7973 (12)	0.7207 (10)	0.063 (5)	0.5
H64A	0.028138	0.834938	0.730485	0.075*	0.5
Cl1A	0.8953 (5)	0.6127 (3)	0.7868 (4)	0.1205 (18)	0.5
C67A	0.7909 (15)	0.6819 (9)	0.7751 (11)	0.089 (5)	0.5
H67C	0.754035	0.673925	0.715656	0.106*	0.5
H67D	0.730772	0.666885	0.802260	0.106*	0.5
Cl2A	0.8538 (6)	0.7886 (4)	0.8186 (5)	0.0798 (17)	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Dy1	0.03374 (11)	0.02867 (10)	0.02777 (10)	0.00470 (7)	0.00846 (7)	0.01536 (7)
O3	0.0318 (15)	0.0272 (14)	0.0420 (16)	0.0066 (11)	0.0114 (12)	0.0073 (12)
O1	0.0308 (14)	0.0308 (14)	0.0332 (14)	0.0102 (11)	0.0103 (12)	0.0135 (11)
O5	0.0273 (13)	0.0333 (14)	0.0291 (14)	0.0066 (11)	0.0117 (11)	0.0129 (11)
O4	0.0470 (17)	0.0343 (15)	0.0275 (14)	0.0137 (13)	0.0155 (13)	0.0076 (12)
O2	0.0242 (14)	0.060 (2)	0.0259 (14)	0.0011 (13)	0.0022 (11)	0.0049 (13)
O6	0.0278 (14)	0.0330 (15)	0.0469 (17)	0.0049 (12)	0.0054 (13)	0.0069 (13)
N2	0.0326 (17)	0.0241 (15)	0.0208 (15)	0.0019 (13)	0.0062 (13)	0.0069 (12)
N8	0.0241 (16)	0.0368 (18)	0.0324 (17)	0.0099 (13)	0.0112 (13)	0.0152 (14)
N5	0.0413 (19)	0.0426 (19)	0.0248 (16)	0.0162 (16)	0.0150 (14)	0.0189 (15)
N7	0.040 (2)	0.055 (2)	0.047 (2)	0.0233 (17)	0.0300 (17)	0.0342 (19)
N1	0.0365 (18)	0.0280 (16)	0.0328 (17)	0.0105 (14)	0.0134 (14)	0.0158 (14)
C61	0.034 (2)	0.0262 (18)	0.0211 (17)	0.0094 (15)	0.0081 (15)	0.0068 (14)
C66	0.024 (4)	0.026 (4)	0.022 (4)	0.005 (3)	0.005 (3)	0.003 (3)
C65	0.035 (4)	0.025 (4)	0.024 (4)	0.004 (3)	0.005 (3)	0.003 (3)
C64	0.028 (7)	0.040 (6)	0.030 (6)	0.022 (5)	0.004 (5)	0.009 (5)
C63	0.028 (4)	0.040 (5)	0.016 (4)	0.014 (3)	0.004 (3)	0.007 (4)
C62	0.029 (4)	0.034 (4)	0.014 (4)	0.006 (3)	0.000 (4)	0.004 (4)
C7	0.042 (2)	0.031 (2)	0.032 (2)	0.0056 (17)	0.0165 (18)	0.0155 (16)
N10	0.0284 (16)	0.0412 (19)	0.0338 (17)	0.0156 (14)	0.0175 (14)	0.0240 (15)
C55	0.0247 (18)	0.0235 (18)	0.035 (2)	0.0048 (14)	0.0102 (16)	0.0099 (15)
C54	0.0268 (18)	0.0245 (18)	0.034 (2)	0.0052 (14)	0.0159 (16)	0.0086 (15)
C21	0.035 (2)	0.0197 (19)	0.075 (3)	0.0047 (16)	0.021 (2)	0.013 (2)
C43	0.0248 (18)	0.0220 (17)	0.0266 (18)	−0.0017 (14)	0.0029 (14)	0.0089 (14)
C4	0.0292 (19)	0.0253 (18)	0.0246 (18)	0.0085 (15)	0.0046 (15)	0.0066 (14)
N12	0.0275 (17)	0.0250 (16)	0.051 (2)	0.0083 (13)	0.0225 (15)	0.0104 (15)
C23	0.043 (3)	0.074 (3)	0.038 (2)	0.026 (2)	0.023 (2)	0.021 (2)
N6	0.0312 (17)	0.0269 (16)	0.0232 (15)	0.0068 (13)	0.0069 (13)	0.0080 (12)
N4	0.0294 (17)	0.0265 (16)	0.0294 (16)	0.0019 (13)	0.0112 (13)	0.0025 (13)
C2	0.032 (2)	0.033 (2)	0.029 (2)	0.0113 (16)	0.0022 (16)	0.0092 (16)
C18	0.026 (2)	0.035 (2)	0.037 (2)	0.0071 (16)	0.0061 (17)	−0.0043 (17)
C25	0.0216 (18)	0.039 (2)	0.0222 (18)	0.0031 (15)	0.0037 (14)	−0.0027 (15)
N3	0.0396 (19)	0.0276 (17)	0.044 (2)	0.0068 (14)	0.0235 (16)	0.0154 (15)
C49	0.0219 (17)	0.0229 (17)	0.0258 (17)	0.0045 (13)	0.0110 (14)	0.0062 (14)
C22	0.053 (3)	0.085 (4)	0.051 (3)	0.035 (3)	0.035 (2)	0.043 (3)
C3	0.0295 (19)	0.0225 (17)	0.0256 (18)	0.0049 (14)	0.0063 (15)	0.0054 (14)
C44	0.032 (2)	0.043 (2)	0.0259 (19)	0.0006 (17)	0.0042 (16)	0.0072 (17)
C26	0.031 (2)	0.046 (3)	0.041 (2)	0.0092 (19)	0.0094 (19)	−0.008 (2)
C35	0.038 (2)	0.034 (2)	0.0264 (19)	−0.0004 (17)	0.0151 (17)	0.0111 (16)
C6	0.041 (2)	0.042 (2)	0.045 (2)	0.0061 (19)	0.024 (2)	0.013 (2)
C24	0.0230 (19)	0.049 (2)	0.031 (2)	0.0114 (17)	0.0092 (16)	0.0126 (18)
N9	0.051 (2)	0.061 (3)	0.061 (3)	0.036 (2)	0.040 (2)	0.049 (2)
C17	0.030 (2)	0.038 (2)	0.0274 (19)	0.0119 (17)	0.0050 (16)	−0.0006 (16)
C32	0.028 (2)	0.043 (2)	0.0284 (19)	0.0105 (17)	0.0099 (16)	0.0101 (17)
C5	0.031 (2)	0.039 (2)	0.048 (3)	0.0135 (18)	0.0157 (19)	0.0160 (19)

C16	0.057 (3)	0.067 (3)	0.022 (2)	0.032 (3)	0.013 (2)	0.004 (2)
C53	0.044 (2)	0.0207 (18)	0.052 (3)	0.0028 (17)	0.027 (2)	0.0064 (17)
N11	0.046 (2)	0.0320 (18)	0.072 (3)	0.0168 (16)	0.044 (2)	0.0291 (18)
C28	0.059 (3)	0.036 (2)	0.052 (3)	0.012 (2)	0.021 (2)	0.016 (2)
C27	0.043 (3)	0.030 (2)	0.067 (3)	0.0078 (19)	0.014 (2)	0.001 (2)
C15	0.062 (3)	0.072 (3)	0.026 (2)	0.036 (3)	0.021 (2)	0.025 (2)
C46	0.047 (3)	0.058 (3)	0.044 (3)	−0.021 (2)	−0.017 (2)	0.035 (2)
C1	0.041 (2)	0.036 (2)	0.042 (2)	0.0140 (18)	0.0113 (19)	0.0213 (19)
C52	0.036 (2)	0.029 (2)	0.051 (3)	−0.0061 (17)	0.022 (2)	−0.0131 (19)
C31	0.035 (2)	0.052 (3)	0.034 (2)	0.0246 (19)	0.0187 (18)	0.0207 (19)
C45	0.050 (3)	0.064 (3)	0.025 (2)	−0.018 (2)	0.0026 (19)	0.014 (2)
C58	0.040 (3)	0.056 (3)	0.082 (4)	0.007 (2)	0.035 (3)	0.038 (3)
C48	0.029 (2)	0.043 (2)	0.044 (2)	0.0073 (18)	0.0062 (18)	0.022 (2)
C51	0.038 (2)	0.044 (3)	0.038 (2)	0.005 (2)	0.0012 (19)	−0.005 (2)
C20	0.031 (2)	0.024 (2)	0.091 (4)	0.0062 (17)	0.016 (2)	−0.003 (2)
C50	0.041 (2)	0.030 (2)	0.035 (2)	0.0090 (18)	−0.0015 (18)	0.0066 (17)
C39	0.027 (2)	0.030 (2)	0.050 (3)	−0.0017 (16)	0.0173 (19)	−0.0134 (18)
C34	0.039 (2)	0.051 (3)	0.040 (2)	0.012 (2)	0.024 (2)	0.014 (2)
C14	0.037 (2)	0.083 (4)	0.028 (2)	0.021 (2)	0.0070 (19)	0.009 (2)
C38	0.035 (2)	0.027 (2)	0.054 (3)	0.0018 (17)	0.028 (2)	−0.0042 (18)
C19	0.034 (2)	0.036 (2)	0.058 (3)	0.0085 (19)	0.006 (2)	−0.015 (2)
B3	0.0222 (19)	0.0193 (18)	0.0256 (19)	0.0033 (15)	0.0071 (16)	0.0068 (15)
C37	0.057 (3)	0.034 (2)	0.090 (4)	−0.003 (2)	0.058 (3)	0.003 (3)
C42	0.038 (2)	0.048 (3)	0.040 (2)	0.013 (2)	−0.0007 (19)	0.000 (2)
C56A	0.018 (5)	0.024 (4)	0.026 (5)	0.006 (3)	0.005 (4)	0.005 (4)
C33	0.038 (2)	0.061 (3)	0.046 (3)	0.025 (2)	0.027 (2)	0.025 (2)
C47	0.034 (2)	0.058 (3)	0.058 (3)	0.004 (2)	−0.003 (2)	0.034 (3)
C11	0.0225 (19)	0.043 (2)	0.039 (2)	−0.0054 (17)	0.0125 (17)	−0.0101 (19)
C9	0.031 (2)	0.027 (2)	0.074 (3)	−0.0077 (17)	0.025 (2)	−0.001 (2)
C12	0.030 (2)	0.071 (4)	0.041 (3)	−0.002 (2)	0.002 (2)	−0.008 (2)
C8	0.040 (2)	0.029 (2)	0.068 (3)	−0.0001 (18)	0.028 (2)	0.015 (2)
C40	0.030 (2)	0.070 (4)	0.051 (3)	−0.009 (2)	0.012 (2)	−0.019 (3)
C13	0.030 (2)	0.097 (4)	0.031 (2)	0.014 (3)	−0.0059 (19)	−0.012 (3)
C41	0.034 (3)	0.080 (4)	0.046 (3)	0.012 (2)	−0.001 (2)	−0.011 (3)
C30	0.062 (3)	0.104 (5)	0.076 (4)	0.072 (3)	0.054 (3)	0.065 (4)
C29	0.088 (4)	0.105 (5)	0.089 (4)	0.076 (4)	0.061 (4)	0.085 (4)
C10	0.028 (2)	0.035 (2)	0.039 (2)	0.0027 (16)	0.0129 (17)	−0.0052 (17)
C57A	0.028 (5)	0.025 (6)	0.032 (5)	0.010 (4)	0.015 (4)	0.008 (4)
B1	0.044 (3)	0.034 (2)	0.039 (3)	0.014 (2)	0.025 (2)	0.024 (2)
C36	0.065 (3)	0.035 (2)	0.090 (4)	0.014 (2)	0.057 (3)	0.026 (3)
C59A	0.032 (4)	0.024 (3)	0.017 (3)	−0.001 (3)	0.007 (3)	0.007 (3)
B2	0.057 (3)	0.058 (3)	0.063 (4)	0.034 (3)	0.044 (3)	0.046 (3)
C60A	0.022 (3)	0.024 (3)	0.020 (3)	0.004 (3)	0.005 (3)	0.010 (3)
Cl2	0.101 (5)	0.0409 (18)	0.068 (3)	0.004 (3)	−0.013 (3)	0.0062 (17)
Cl1	0.0604 (18)	0.0497 (16)	0.102 (2)	0.0203 (13)	0.0216 (17)	0.0296 (15)
C67	0.070 (7)	0.037 (5)	0.080 (8)	0.014 (5)	−0.018 (6)	0.008 (5)
C60	0.046 (5)	0.040 (5)	0.052 (6)	−0.007 (4)	0.028 (5)	0.001 (4)
C59	0.061 (7)	0.044 (6)	0.065 (7)	−0.012 (5)	0.034 (6)	0.008 (5)

C57	0.057 (9)	0.036 (7)	0.040 (7)	0.008 (5)	0.032 (7)	0.004 (5)
C56	0.040 (7)	0.034 (6)	0.033 (6)	−0.006 (5)	0.016 (5)	0.003 (4)
C66A	0.059 (6)	0.038 (5)	0.031 (5)	0.016 (4)	0.006 (4)	0.007 (4)
C62A	0.028 (5)	0.039 (5)	0.043 (6)	0.010 (4)	−0.007 (4)	−0.024 (5)
C65A	0.099 (10)	0.037 (5)	0.045 (6)	0.036 (6)	0.017 (7)	0.016 (5)
C63A	0.037 (6)	0.091 (10)	0.036 (6)	0.029 (6)	−0.004 (5)	−0.021 (6)
C64A	0.058 (10)	0.096 (12)	0.034 (7)	0.055 (9)	0.003 (6)	0.006 (7)
Cl1A	0.105 (3)	0.071 (2)	0.196 (6)	0.000 (2)	0.031 (3)	0.071 (3)
C67A	0.089 (10)	0.053 (8)	0.116 (12)	−0.007 (7)	0.017 (8)	0.025 (7)
Cl2A	0.088 (4)	0.063 (3)	0.077 (3)	−0.012 (3)	0.009 (3)	0.018 (3)

Geometric parameters (Å, º)

Dy1—O3	2.755 (3)	N9—B2	1.532 (6)
Dy1—O1	3.181 (3)	C17—C16	1.400 (6)
Dy1—O5	2.775 (3)	C32—C31	1.439 (6)
Dy1—O4	3.102 (3)	C32—C33	1.345 (6)
Dy1—O2	2.887 (3)	C5—H5	0.9500
Dy1—O6	2.995 (3)	C16—H16	0.9500
Dy1—N2	2.626 (3)	C16—C15	1.362 (7)
Dy1—N8	2.573 (3)	C53—H53	0.9500
Dy1—N10	2.489 (3)	C53—C52	1.376 (7)
Dy1—N12	2.555 (3)	N11—C36	1.349 (6)
Dy1—N6	2.525 (3)	N11—B2	1.523 (8)
Dy1—N4	2.532 (3)	C28—H28	0.9500
O3—C21	1.383 (5)	C28—C27	1.350 (7)
O3—C18	1.380 (5)	C27—H27	0.9500
O1—C7	1.386 (5)	C15—H15	0.9500
O1—C4	1.364 (4)	C46—H46	0.9500
O5—C35	1.381 (4)	C46—C45	1.367 (8)
O5—C32	1.370 (5)	C46—C47	1.370 (8)
O4—C25	1.356 (5)	C1—H1	0.9500
O4—C28	1.366 (5)	C52—H52	0.9500
O2—C14	1.376 (5)	C52—C51	1.376 (7)
O2—C11	1.379 (5)	C31—C30	1.390 (6)
O6—C39	1.368 (5)	C45—H45	0.9500
O6—C42	1.364 (6)	C58—H58A	0.9500
N2—N1	1.366 (4)	C58—H58	0.9500
N2—C3	1.352 (5)	C58—C57A	1.464 (12)
N8—N7	1.368 (4)	C58—C59A	1.302 (9)
N8—C24	1.357 (5)	C58—C59	1.586 (12)
N5—N6	1.363 (4)	C58—C57	1.185 (16)
N5—C15	1.348 (5)	C48—H48	0.9500
N5—B1	1.527 (6)	C48—C47	1.386 (6)
N7—C22	1.351 (6)	C51—H51	0.9500
N7—B2	1.533 (7)	C51—C50	1.392 (6)
N1—C1	1.350 (5)	C20—H20	0.9500
N1—B1	1.538 (6)	C20—C19	1.417 (8)

C61—C66	1.3900	C50—H50	0.9500
C61—C62	1.3900	C39—C38	1.429 (7)
C61—B3	1.662 (5)	C39—C40	1.345 (7)
C61—C66A	1.367 (10)	C34—H34	0.9500
C61—C62A	1.407 (12)	C34—C33	1.426 (6)
C66—H66	0.9500	C14—H14	0.9500
C66—C65	1.3900	C14—C13	1.355 (7)
C65—H65	0.9500	C38—C37	1.392 (6)
C65—C64	1.3900	C19—H19	0.9500
C64—H64	0.9500	C37—H37	0.9500
C64—C63	1.3900	C37—C36	1.364 (9)
C63—H63	0.9500	C42—H42	0.9500
C63—C62	1.3900	C42—C41	1.350 (7)
C62—H62	0.9500	C56A—H56A	0.9500
C7—H7	0.9500	C56A—C57A	1.379 (17)
C7—C6	1.317 (6)	C33—H33	0.9500
N10—N9	1.364 (4)	C47—H47	0.9500
N10—C31	1.341 (5)	C11—C12	1.342 (6)
C55—B3	1.653 (5)	C11—C10	1.427 (7)
C55—C56A	1.449 (11)	C9—H9	0.9500
C55—C60A	1.415 (8)	C9—C8	1.354 (7)
C55—C60	1.449 (10)	C9—C10	1.402 (6)
C55—C56	1.296 (12)	C12—H12	0.9500
C54—H54	0.9500	C12—C13	1.398 (8)
C54—C49	1.389 (5)	C8—H8	0.9500
C54—C53	1.392 (5)	C40—H40	0.9500
C21—H21	0.9500	C40—C41	1.413 (9)
C21—C20	1.334 (7)	C13—H13	0.9500
C43—C44	1.400 (5)	C41—H41	0.9500
C43—C48	1.393 (5)	C30—H30	0.9500
C43—B3	1.646 (5)	C30—C29	1.376 (7)
C4—C3	1.440 (5)	C29—H29	0.9500
C4—C5	1.368 (6)	C57A—H57A	0.9500
N12—N11	1.372 (5)	B1—H1A	1.08 (4)
N12—C38	1.339 (6)	C36—H36	0.9500
C23—H23	0.9500	C59A—H59A	0.9500
C23—C22	1.362 (8)	C59A—C60A	1.394 (10)
C23—C24	1.396 (6)	B2—H2A	1.12 (5)
N6—C17	1.347 (5)	C60A—H60A	1.01 (11)
N4—N3	1.371 (5)	Cl2—C67	1.726 (13)
N4—C10	1.341 (5)	Cl1—C67	1.768 (12)
C2—H2	0.9500	C67—H67A	0.9900
C2—C3	1.405 (5)	C67—H67B	0.9900
C2—C1	1.373 (6)	C60—H60	0.9500
C18—C17	1.433 (6)	C60—C59	1.400 (13)
C18—C19	1.348 (6)	C59—H59	0.9500
C25—C26	1.350 (6)	C57—H57	0.9500
C25—C24	1.437 (6)	C57—C56	1.418 (18)

N3—C8	1.345 (5)	C56—H56	0.9500
N3—B1	1.523 (6)	C66A—H66A	0.9500
C49—C50	1.397 (5)	C66A—C65A	1.423 (15)
C49—B3	1.652 (5)	C62A—H62A	0.81 (11)
C22—H22	0.9500	C62A—C63A	1.403 (14)
C44—H44	0.9500	C65A—H65A	0.9500
C44—C45	1.394 (6)	C65A—C64A	1.33 (2)
C26—H26	0.9500	C63A—H63A	0.9500
C26—C27	1.417 (7)	C63A—C64A	1.37 (2)
C35—H35	0.9500	C64A—H64A	0.9500
C35—C34	1.334 (6)	Cl1A—C67A	1.784 (18)
C6—H6	0.9500	C67A—H67C	0.9900
C6—C5	1.421 (6)	C67A—H67D	0.9900
N9—C29	1.342 (6)	C67A—Cl2A	1.738 (15)

O3—Dy1—O1	115.13 (8)	N10—N9—B2	121.7 (3)
O3—Dy1—O5	64.13 (8)	C29—N9—N10	109.8 (4)
O3—Dy1—O4	177.12 (8)	C29—N9—B2	128.5 (4)
O3—Dy1—O2	119.60 (9)	N6—C17—C18	119.0 (4)
O3—Dy1—O6	62.60 (8)	N6—C17—C16	110.6 (4)
O5—Dy1—O1	178.72 (7)	C16—C17—C18	130.4 (4)
O5—Dy1—O4	116.79 (8)	O5—C32—C31	114.2 (3)
O5—Dy1—O2	64.52 (8)	C33—C32—O5	110.0 (4)
O5—Dy1—O6	117.52 (8)	C33—C32—C31	135.9 (4)
O4—Dy1—O1	64.00 (7)	C4—C5—C6	105.9 (4)
O2—Dy1—O1	115.51 (8)	C4—C5—H5	127.1
O2—Dy1—O4	62.74 (8)	C6—C5—H5	127.1
O2—Dy1—O6	177.76 (8)	C17—C16—H16	127.6
O6—Dy1—O1	62.47 (8)	C15—C16—C17	104.7 (4)
O6—Dy1—O4	115.07 (8)	C15—C16—H16	127.6
N2—Dy1—O3	117.32 (9)	C54—C53—H53	119.8
N2—Dy1—O1	55.19 (8)	C52—C53—C54	120.4 (4)
N2—Dy1—O5	126.02 (9)	C52—C53—H53	119.8
N2—Dy1—O4	59.84 (8)	N12—N11—B2	122.9 (3)
N2—Dy1—O2	117.65 (9)	C36—N11—N12	110.5 (4)
N2—Dy1—O6	60.57 (9)	C36—N11—B2	126.6 (4)
N8—Dy1—O3	125.78 (10)	O4—C28—H28	124.7
N8—Dy1—O1	57.78 (8)	C27—C28—O4	110.5 (4)
N8—Dy1—O5	121.63 (9)	C27—C28—H28	124.7
N8—Dy1—O4	56.41 (9)	C26—C27—H27	127.0
N8—Dy1—O2	63.62 (9)	C28—C27—C26	106.0 (4)
N8—Dy1—O6	114.98 (9)	C28—C27—H27	127.0
N8—Dy1—N2	100.86 (10)	N5—C15—C16	109.0 (4)
N10—Dy1—O3	65.01 (10)	N5—C15—H15	125.5
N10—Dy1—O1	118.47 (8)	C16—C15—H15	125.5
N10—Dy1—O5	60.33 (9)	C45—C46—H46	120.5
N10—Dy1—O4	117.86 (10)	C45—C46—C47	119.1 (4)
N10—Dy1—O2	63.21 (11)	C47—C46—H46	120.5

N10—Dy1—O6	118.39 (10)	N1—C1—C2	109.5 (4)
N10—Dy1—N2	173.61 (10)	N1—C1—H1	125.2
N10—Dy1—N8	73.65 (10)	C2—C1—H1	125.2
N10—Dy1—N12	72.41 (11)	C53—C52—H52	120.5
N10—Dy1—N6	114.46 (10)	C51—C52—C53	118.9 (4)
N10—Dy1—N4	112.09 (11)	C51—C52—H52	120.5
N12—Dy1—O3	64.74 (9)	N10—C31—C32	119.2 (4)
N12—Dy1—O1	58.05 (8)	N10—C31—C30	111.2 (4)
N12—Dy1—O5	120.77 (9)	C30—C31—C32	129.6 (4)
N12—Dy1—O4	115.80 (9)	C44—C45—H45	119.9
N12—Dy1—O2	122.60 (10)	C46—C45—C44	120.3 (5)
N12—Dy1—O6	57.52 (10)	C46—C45—H45	119.9
N12—Dy1—N2	102.88 (10)	C57A—C58—H58A	119.4
N12—Dy1—N8	70.53 (11)	C59A—C58—H58A	119.4
N6—Dy1—O3	59.91 (9)	C59A—C58—C57A	121.2 (7)
N6—Dy1—O1	115.25 (9)	C59—C58—H58	123.1
N6—Dy1—O5	65.43 (9)	C57—C58—H58	123.1
N6—Dy1—O4	117.70 (9)	C57—C58—C59	113.7 (8)
N6—Dy1—O2	120.11 (9)	C43—C48—H48	118.6
N6—Dy1—O6	61.03 (9)	C47—C48—C43	122.8 (4)
N6—Dy1—N2	70.99 (10)	C47—C48—H48	118.6
N6—Dy1—N8	171.83 (10)	C52—C51—H51	120.1
N6—Dy1—N12	110.20 (11)	C52—C51—C50	119.9 (4)
N6—Dy1—N4	71.42 (10)	C50—C51—H51	120.1
N4—Dy1—O3	119.86 (9)	C21—C20—H20	126.3
N4—Dy1—O1	116.36 (9)	C21—C20—C19	107.4 (4)
N4—Dy1—O5	64.83 (9)	C19—C20—H20	126.3
N4—Dy1—O4	59.43 (9)	C49—C50—H50	118.5
N4—Dy1—O2	58.89 (10)	C51—C50—C49	122.9 (4)
N4—Dy1—O6	120.74 (10)	C51—C50—H50	118.5
N4—Dy1—N2	72.36 (10)	O6—C39—C38	115.8 (4)
N4—Dy1—N8	107.08 (10)	C40—C39—O6	109.8 (5)
N4—Dy1—N12	174.40 (10)	C40—C39—C38	134.4 (5)
C21—O3—Dy1	133.3 (3)	C35—C34—H34	126.4
C18—O3—Dy1	120.1 (2)	C35—C34—C33	107.3 (4)
C18—O3—C21	106.5 (3)	C33—C34—H34	126.4
C7—O1—Dy1	138.7 (2)	O2—C14—H14	125.6
C4—O1—Dy1	114.9 (2)	C13—C14—O2	108.9 (5)
C4—O1—C7	105.8 (3)	C13—C14—H14	125.6
C35—O5—Dy1	134.8 (2)	N12—C38—C39	119.9 (4)
C32—O5—Dy1	118.5 (2)	N12—C38—C37	110.7 (5)
C32—O5—C35	106.5 (3)	C37—C38—C39	129.4 (5)
C25—O4—Dy1	113.7 (2)	C18—C19—C20	107.2 (4)
C25—O4—C28	106.3 (3)	C18—C19—H19	126.4
C28—O4—Dy1	134.7 (3)	C20—C19—H19	126.4
C14—O2—Dy1	135.5 (3)	C55—B3—C61	111.2 (3)
C14—O2—C11	106.7 (4)	C43—B3—C61	108.6 (3)
C11—O2—Dy1	116.8 (2)	C43—B3—C55	109.8 (3)

C39—O6—Dy1	115.3 (3)	C43—B3—C49	108.7 (3)
C42—O6—Dy1	136.7 (3)	C49—B3—C61	111.3 (3)
C42—O6—C39	107.1 (4)	C49—B3—C55	107.2 (3)
N1—N2—Dy1	122.6 (2)	C38—C37—H37	127.2
C3—N2—Dy1	132.5 (2)	C36—C37—C38	105.7 (5)
C3—N2—N1	104.9 (3)	C36—C37—H37	127.2
N7—N8—Dy1	123.9 (3)	O6—C42—H42	125.4
C24—N8—Dy1	131.1 (3)	C41—C42—O6	109.2 (5)
C24—N8—N7	105.0 (3)	C41—C42—H42	125.4
N6—N5—B1	120.9 (3)	C55—C56A—H56A	117.5
C15—N5—N6	110.1 (4)	C57A—C56A—C55	125.1 (9)
C15—N5—B1	128.9 (4)	C57A—C56A—H56A	117.5
N8—N7—B2	122.3 (3)	C32—C33—C34	106.5 (4)
C22—N7—N8	110.3 (4)	C32—C33—H33	126.7
C22—N7—B2	127.2 (4)	C34—C33—H33	126.7
N2—N1—B1	123.3 (3)	C46—C47—C48	120.5 (5)
C1—N1—N2	110.3 (3)	C46—C47—H47	119.8
C1—N1—B1	126.2 (3)	C48—C47—H47	119.8
C66—C61—C62	120.0	O2—C11—C10	114.5 (3)
C66—C61—B3	115.5 (3)	C12—C11—O2	109.3 (5)
C62—C61—B3	124.5 (3)	C12—C11—C10	136.1 (5)
C66A—C61—B3	128.1 (5)	C8—C9—H9	127.3
C66A—C61—C62A	111.7 (7)	C8—C9—C10	105.4 (4)
C62A—C61—B3	119.6 (5)	C10—C9—H9	127.3
C61—C66—H66	120.0	C11—C12—H12	126.2
C61—C66—C65	120.0	C11—C12—C13	107.6 (5)
C65—C66—H66	120.0	C13—C12—H12	126.2
C66—C65—H65	120.0	N3—C8—C9	108.7 (4)
C64—C65—C66	120.0	N3—C8—H8	125.6
C64—C65—H65	120.0	C9—C8—H8	125.6
C65—C64—H64	120.0	C39—C40—H40	126.7
C63—C64—C65	120.0	C39—C40—C41	106.5 (5)
C63—C64—H64	120.0	C41—C40—H40	126.7
C64—C63—H63	120.0	C14—C13—C12	107.5 (4)
C64—C63—C62	120.0	C14—C13—H13	126.3
C62—C63—H63	120.0	C12—C13—H13	126.3
C61—C62—H62	120.0	C42—C41—C40	107.3 (5)
C63—C62—C61	120.0	C42—C41—H41	126.3
C63—C62—H62	120.0	C40—C41—H41	126.3
O1—C7—H7	124.6	C31—C30—H30	127.9
C6—C7—O1	110.7 (4)	C29—C30—C31	104.2 (4)
C6—C7—H7	124.6	C29—C30—H30	127.9
N9—N10—Dy1	126.6 (2)	N9—C29—C30	109.1 (4)
C31—N10—Dy1	127.6 (3)	N9—C29—H29	125.5
C31—N10—N9	105.7 (3)	C30—C29—H29	125.5
C56A—C55—B3	121.8 (5)	N4—C10—C11	120.4 (4)
C60A—C55—B3	126.3 (4)	N4—C10—C9	110.3 (4)
C60A—C55—C56A	111.5 (6)	C9—C10—C11	129.3 (4)

C60—C55—B3	115.8 (5)	C58—C57A—H57A	122.2
C56—C55—B3	126.2 (6)	C56A—C57A—C58	115.6 (9)
C56—C55—C60	117.2 (7)	C56A—C57A—H57A	122.2
C49—C54—H54	118.7	N5—B1—N1	108.5 (3)
C49—C54—C53	122.6 (4)	N5—B1—H1A	112 (2)
C53—C54—H54	118.7	N1—B1—H1A	107 (2)
O3—C21—H21	125.2	N3—B1—N5	108.7 (3)
C20—C21—O3	109.7 (5)	N3—B1—N1	110.3 (3)
C20—C21—H21	125.2	N3—B1—H1A	110 (2)
C44—C43—B3	122.4 (3)	N11—C36—C37	107.9 (4)
C48—C43—C44	114.9 (4)	N11—C36—H36	126.1
C48—C43—B3	122.5 (3)	C37—C36—H36	126.1
O1—C4—C3	115.0 (3)	C58—C59A—H59A	120.1
O1—C4—C5	110.0 (3)	C58—C59A—C60A	119.8 (6)
C5—C4—C3	135.0 (4)	C60A—C59A—H59A	120.1
N11—N12—Dy1	123.8 (3)	N7—B2—H2A	112 (2)
C38—N12—Dy1	130.9 (3)	N9—B2—N7	109.2 (4)
C38—N12—N11	105.3 (3)	N9—B2—H2A	108 (2)
C22—C23—H23	127.6	N11—B2—N7	108.8 (4)
C22—C23—C24	104.9 (4)	N11—B2—N9	108.6 (4)
C24—C23—H23	127.6	N11—B2—H2A	110 (2)
N5—N6—Dy1	127.2 (2)	C55—C60A—H60A	115 (6)
C17—N6—Dy1	127.1 (3)	C59A—C60A—C55	124.7 (6)
C17—N6—N5	105.5 (3)	C59A—C60A—H60A	120 (6)
N3—N4—Dy1	125.9 (2)	Cl2—C67—Cl1	113.2 (7)
C10—N4—Dy1	128.5 (3)	Cl2—C67—H67A	108.9
C10—N4—N3	105.5 (3)	Cl2—C67—H67B	108.9
C3—C2—H2	128.2	Cl1—C67—H67A	108.9
C1—C2—H2	128.2	Cl1—C67—H67B	108.9
C1—C2—C3	103.5 (3)	H67A—C67—H67B	107.8
O3—C18—C17	113.7 (3)	C55—C60—H60	120.5
C19—C18—O3	109.2 (4)	C59—C60—C55	118.9 (8)
C19—C18—C17	137.0 (5)	C59—C60—H60	120.5
O4—C25—C24	114.8 (3)	C58—C59—H59	121.0
C26—C25—O4	110.4 (4)	C60—C59—C58	118.0 (8)
C26—C25—C24	134.8 (4)	C60—C59—H59	121.0
N4—N3—B1	122.0 (3)	C58—C57—H57	116.3
C8—N3—N4	110.1 (4)	C58—C57—C56	127.3 (12)
C8—N3—B1	127.8 (4)	C56—C57—H57	116.3
C54—C49—C50	115.2 (3)	C55—C56—C57	122.9 (10)
C54—C49—B3	124.0 (3)	C55—C56—H56	118.5
C50—C49—B3	120.7 (3)	C57—C56—H56	118.5
N7—C22—C23	109.0 (4)	C61—C66A—H66A	118.5
N7—C22—H22	125.5	C61—C66A—C65A	123.1 (10)
C23—C22—H22	125.5	C65A—C66A—H66A	118.5
N2—C3—C4	121.9 (3)	C61—C62A—H62A	119 (8)
N2—C3—C2	111.7 (3)	C63A—C62A—C61	124.2 (11)
C2—C3—C4	126.3 (4)	C63A—C62A—H62A	117 (8)

C43—C44—H44	118.8	C66A—C65A—H65A	118.2
C45—C44—C43	122.4 (4)	C64A—C65A—C66A	123.6 (12)
C45—C44—H44	118.8	C64A—C65A—H65A	118.2
C25—C26—H26	126.6	C62A—C63A—H63A	119.3
C25—C26—C27	106.8 (4)	C64A—C63A—C62A	121.4 (14)
C27—C26—H26	126.6	C64A—C63A—H63A	119.3
O5—C35—H35	125.1	C65A—C64A—C63A	115.4 (12)
C34—C35—O5	109.7 (4)	C65A—C64A—H64A	122.3
C34—C35—H35	125.1	C63A—C64A—H64A	122.3
C7—C6—H6	126.2	Cl1A—C67A—H67C	109.5
C7—C6—C5	107.6 (4)	Cl1A—C67A—H67D	109.5
C5—C6—H6	126.2	H67C—C67A—H67D	108.1
N8—C24—C23	110.9 (4)	Cl2A—C67A—Cl1A	110.8 (10)
N8—C24—C25	120.9 (3)	Cl2A—C67A—H67C	109.5
C23—C24—C25	128.1 (4)	Cl2A—C67A—H67D	109.5

Dy1—O3—C21—C20	−176.7 (3)	C3—C2—C1—N1	−0.7 (5)
Dy1—O3—C18—C17	−1.9 (4)	C44—C43—C48—C47	1.2 (6)
Dy1—O3—C18—C19	177.3 (3)	C44—C43—B3—C61	29.4 (5)
Dy1—O1—C7—C6	169.2 (3)	C44—C43—B3—C55	151.2 (3)
Dy1—O1—C4—C3	7.2 (4)	C44—C43—B3—C49	−91.8 (4)
Dy1—O1—C4—C5	−172.6 (3)	C26—C25—C24—N8	−162.4 (4)
Dy1—O5—C35—C34	174.9 (3)	C26—C25—C24—C23	15.4 (8)
Dy1—O5—C32—C31	4.1 (5)	C35—O5—C32—C31	−179.6 (4)
Dy1—O5—C32—C33	−175.7 (3)	C35—O5—C32—C33	0.6 (5)
Dy1—O4—C25—C26	158.9 (3)	C35—C34—C33—C32	0.1 (6)
Dy1—O4—C25—C24	−19.3 (4)	C24—N8—N7—C22	0.2 (5)
Dy1—O4—C28—C27	−152.6 (3)	C24—N8—N7—B2	−174.4 (4)
Dy1—O2—C14—C13	−167.3 (3)	C24—C23—C22—N7	0.1 (6)
Dy1—O2—C11—C12	170.1 (3)	C24—C25—C26—C27	177.7 (4)
Dy1—O2—C11—C10	−9.7 (4)	N9—N10—C31—C32	−179.9 (4)
Dy1—O6—C39—C38	8.6 (4)	N9—N10—C31—C30	−0.1 (6)
Dy1—O6—C39—C40	−171.5 (3)	C17—C18—C19—C20	178.7 (5)
Dy1—O6—C42—C41	168.6 (3)	C17—C16—C15—N5	0.2 (6)
Dy1—N2—N1—C1	−176.3 (3)	C32—O5—C35—C34	−0.5 (5)
Dy1—N2—N1—B1	−0.9 (5)	C32—C31—C30—C29	−180.0 (6)
Dy1—N2—C3—C4	−3.1 (5)	C5—C4—C3—N2	175.7 (4)
Dy1—N2—C3—C2	175.5 (2)	C5—C4—C3—C2	−2.7 (7)
Dy1—N8—N7—C22	178.7 (3)	C53—C54—C49—C50	0.5 (5)
Dy1—N8—N7—B2	4.1 (5)	C53—C54—C49—B3	−176.4 (3)
Dy1—N8—C24—C23	−178.5 (3)	C53—C52—C51—C50	−1.4 (7)
Dy1—N8—C24—C25	−0.4 (5)	N11—N12—C38—C39	−177.7 (3)
Dy1—N10—N9—C29	177.0 (4)	N11—N12—C38—C37	0.6 (4)
Dy1—N10—N9—B2	−3.8 (7)	C28—O4—C25—C26	0.5 (5)
Dy1—N10—C31—C32	3.0 (6)	C28—O4—C25—C24	−177.7 (4)
Dy1—N10—C31—C30	−177.2 (4)	C15—N5—N6—Dy1	176.7 (3)
Dy1—N12—N11—C36	177.9 (3)	C15—N5—N6—C17	−0.2 (5)
Dy1—N12—N11—B2	−5.2 (5)	C15—N5—B1—N1	−115.0 (5)

Dy1—N12—C38—C39	4.1 (5)	C15—N5—B1—N3	125.0 (5)
Dy1—N12—C38—C37	−177.6 (3)	C1—N1—B1—N5	115.1 (4)
Dy1—N6—C17—C18	3.1 (5)	C1—N1—B1—N3	−125.9 (4)
Dy1—N6—C17—C16	−176.6 (3)	C1—C2—C3—N2	1.3 (5)
Dy1—N4—N3—C8	176.1 (3)	C1—C2—C3—C4	179.8 (4)
Dy1—N4—N3—B1	−1.6 (5)	C52—C51—C50—C49	−0.4 (7)
Dy1—N4—C10—C11	3.9 (5)	C31—N10—N9—C29	−0.1 (6)
Dy1—N4—C10—C9	−175.4 (3)	C31—N10—N9—B2	179.1 (5)
O3—C21—C20—C19	0.2 (5)	C31—C32—C33—C34	179.8 (5)
O3—C18—C17—N6	−0.5 (5)	C31—C30—C29—N9	−0.3 (8)
O3—C18—C17—C16	179.2 (4)	C45—C46—C47—C48	−0.1 (8)
O3—C18—C19—C20	−0.2 (5)	C58—C59A—C60A—C55	−1.1 (11)
O1—C7—C6—C5	1.0 (5)	C58—C57—C56—C55	−8 (2)
O1—C4—C3—N2	−4.0 (5)	C48—C43—C44—C45	−0.6 (6)
O1—C4—C3—C2	177.7 (4)	C48—C43—B3—C61	−155.1 (3)
O1—C4—C5—C6	0.5 (5)	C48—C43—B3—C55	−33.4 (5)
O5—C35—C34—C33	0.2 (5)	C48—C43—B3—C49	83.6 (4)
O5—C32—C31—N10	−4.6 (6)	C50—C49—B3—C61	48.2 (5)
O5—C32—C31—C30	175.6 (5)	C50—C49—B3—C55	−73.6 (4)
O5—C32—C33—C34	−0.4 (5)	C50—C49—B3—C43	167.7 (3)
O4—C25—C26—C27	0.0 (5)	C39—O6—C42—C41	0.3 (5)
O4—C25—C24—N8	15.2 (5)	C39—C38—C37—C36	177.6 (4)
O4—C25—C24—C23	−167.0 (4)	C39—C40—C41—C42	−0.1 (6)
O4—C28—C27—C26	0.9 (6)	C14—O2—C11—C12	−0.1 (5)
O2—C14—C13—C12	−0.2 (6)	C14—O2—C11—C10	−179.9 (4)
O2—C11—C12—C13	0.0 (5)	C38—N12—N11—C36	−0.4 (4)
O2—C11—C10—N4	4.9 (5)	C38—N12—N11—B2	176.4 (4)
O2—C11—C10—C9	−175.9 (4)	C38—C39—C40—C41	−179.9 (5)
O6—C39—C38—N12	−8.7 (5)	C38—C37—C36—N11	0.2 (5)
O6—C39—C38—C37	173.4 (4)	C19—C18—C17—N6	−179.4 (5)
O6—C39—C40—C41	0.3 (5)	C19—C18—C17—C16	0.3 (9)
O6—C42—C41—C40	−0.1 (6)	B3—C61—C66—C65	−178.4 (3)
N2—N1—C1—C2	−0.1 (5)	B3—C61—C62—C63	178.2 (4)
N2—N1—B1—N5	−59.6 (5)	B3—C61—C66A—C65A	−179.4 (7)
N2—N1—B1—N3	59.3 (5)	B3—C61—C62A—C63A	178.9 (9)
N8—N7—C22—C23	−0.2 (6)	B3—C55—C56A—C57A	−179.8 (8)
N8—N7—B2—N9	−60.8 (6)	B3—C55—C60A—C59A	179.0 (6)
N8—N7—B2—N11	57.5 (5)	B3—C55—C60—C59	178.7 (9)
N5—N6—C17—C18	−180.0 (3)	B3—C55—C56—C57	−175.0 (9)
N5—N6—C17—C16	0.3 (5)	B3—C43—C44—C45	175.1 (4)
N7—N8—C24—C23	−0.1 (4)	B3—C43—C48—C47	−174.5 (4)
N7—N8—C24—C25	178.0 (3)	B3—C49—C50—C51	177.9 (4)
N1—N2—C3—C4	−179.9 (3)	C42—O6—C39—C38	179.8 (3)
N1—N2—C3—C2	−1.3 (4)	C42—O6—C39—C40	−0.3 (5)
C61—C66—C65—C64	0.0	C56A—C55—B3—C61	−160.8 (5)
C61—C66A—C65A—C64A	−5.1 (18)	C56A—C55—B3—C43	79.0 (6)
C61—C62A—C63A—C64A	4.1 (19)	C56A—C55—B3—C49	−39.0 (6)
C66—C61—C62—C63	0.0	C56A—C55—C60A—C59A	−9.2 (9)

C66—C61—B3—C55	−58.3 (4)	C33—C32—C31—N10	175.1 (5)
C66—C61—B3—C43	62.6 (4)	C33—C32—C31—C30	−4.6 (10)
C66—C61—B3—C49	−177.7 (3)	C47—C46—C45—C44	0.6 (7)
C66—C65—C64—C63	0.0	C11—O2—C14—C13	0.2 (5)
C65—C64—C63—C62	0.0	C11—C12—C13—C14	0.1 (6)
C64—C63—C62—C61	0.0	C12—C11—C10—N4	−174.8 (5)
C62—C61—C66—C65	0.0	C12—C11—C10—C9	4.3 (8)
C62—C61—B3—C55	123.4 (3)	C8—N3—B1—N5	−117.2 (4)
C62—C61—B3—C43	−115.7 (3)	C8—N3—B1—N1	124.0 (4)
C62—C61—B3—C49	4.0 (4)	C8—C9—C10—N4	−1.1 (5)
C7—O1—C4—C3	179.8 (3)	C8—C9—C10—C11	179.7 (4)
C7—O1—C4—C5	0.1 (4)	C40—C39—C38—N12	171.4 (5)
C7—C6—C5—C4	−0.9 (5)	C40—C39—C38—C37	−6.5 (8)
N10—N9—C29—C30	0.2 (8)	C29—N9—B2—N7	−119.5 (6)
N10—N9—B2—N7	61.6 (6)	C29—N9—B2—N11	122.0 (6)
N10—N9—B2—N11	−56.9 (6)	C10—N4—N3—C8	−0.2 (4)
N10—C31—C30—C29	0.2 (7)	C10—N4—N3—B1	−178.0 (3)
C55—C56A—C57A—C58	2.8 (15)	C10—C11—C12—C13	179.8 (5)
C55—C60—C59—C58	−0.5 (15)	C10—C9—C8—N3	0.9 (5)
C54—C49—C50—C51	0.9 (6)	C57A—C58—C59A—C60A	13.6 (11)
C54—C49—B3—C61	−135.1 (3)	B1—N5—N6—Dy1	0.2 (5)
C54—C49—B3—C55	103.1 (4)	B1—N5—N6—C17	−176.7 (4)
C54—C49—B3—C43	−15.5 (5)	B1—N5—C15—C16	176.2 (4)
C54—C53—C52—C51	2.7 (6)	B1—N1—C1—C2	−175.4 (4)
C21—O3—C18—C17	−178.9 (3)	B1—N3—C8—C9	177.1 (4)
C21—O3—C18—C19	0.3 (4)	C36—N11—B2—N7	119.1 (4)
C21—C20—C19—C18	0.0 (5)	C36—N11—B2—N9	−122.1 (4)
C43—C44—C45—C46	−0.3 (7)	C59A—C58—C57A—C56A	−14.3 (13)
C43—C48—C47—C46	−0.9 (7)	B2—N7—C22—C23	174.1 (5)
C4—O1—C7—C6	−0.7 (5)	B2—N9—C29—C30	−178.8 (6)
N12—N11—C36—C37	0.1 (5)	B2—N11—C36—C37	−176.6 (4)
N12—N11—B2—N7	−57.2 (5)	C60A—C55—B3—C61	10.2 (6)
N12—N11—B2—N9	61.6 (5)	C60A—C55—B3—C43	−110.0 (5)
N12—C38—C37—C36	−0.5 (5)	C60A—C55—B3—C49	132.1 (5)
N6—N5—C15—C16	0.0 (5)	C60A—C55—C56A—C57A	7.9 (12)
N6—N5—B1—N1	60.8 (5)	C60—C55—B3—C61	61.6 (6)
N6—N5—B1—N3	−59.2 (5)	C60—C55—B3—C43	−58.6 (6)
N6—C17—C16—C15	−0.3 (5)	C60—C55—B3—C49	−176.5 (6)
N4—N3—C8—C9	−0.5 (5)	C60—C55—C56—C57	−6.2 (16)
N4—N3—B1—N5	60.1 (4)	C59—C58—C57—C56	15.6 (19)
N4—N3—B1—N1	−58.7 (5)	C57—C58—C59—C60	−11.3 (15)
C18—O3—C21—C20	−0.3 (5)	C56—C55—B3—C61	−129.5 (8)
C18—C17—C16—C15	−180.0 (4)	C56—C55—B3—C43	110.3 (8)
C25—O4—C28—C27	−0.9 (5)	C56—C55—B3—C49	−7.7 (8)
C25—C26—C27—C28	−0.5 (5)	C56—C55—C60—C59	8.8 (14)
N3—N4—C10—C11	−179.9 (3)	C66A—C61—B3—C55	−12.9 (7)
N3—N4—C10—C9	0.8 (4)	C66A—C61—B3—C43	108.1 (6)
C49—C54—C53—C52	−2.3 (6)	C66A—C61—B3—C49	−132.3 (6)

C22—N7—B2—N9	125.5 (5)	C66A—C61—C62A—C63A	−9.1 (12)
C22—N7—B2—N11	−116.1 (5)	C66A—C65A—C64A—C63A	−1 (2)
C22—C23—C24—N8	0.0 (5)	C62A—C61—B3—C55	157.7 (6)
C22—C23—C24—C25	−177.9 (4)	C62A—C61—B3—C43	−81.4 (6)
C3—N2—N1—C1	0.9 (4)	C62A—C61—B3—C49	38.2 (6)
C3—N2—N1—B1	176.3 (4)	C62A—C61—C66A—C65A	9.5 (11)
C3—C4—C5—C6	−179.2 (4)	C62A—C63A—C64A—C65A	1 (2)

Bis{hydrobis[3-(2-furyl)pyrazol-1-yl][5-(2-furyl)pyrazol-1-yl]borato}dysprosium(III) tetraphenylborate (2)

Crystal data

$[Dy(C_{21}H_{16}BN_6O_3)_2](C_{24}H_{20}B)$
M_r = 1304.12
Triclinic, $P\overline{1}$
a = 11.7200 (4) Å
b = 11.9389 (5) Å
c = 21.9139 (9) Å
α = 75.579 (2)°
β = 76.715 (1)°
γ = 86.477 (1)°
V = 2890.2 (2) Å^3
Z = 2
$F(000)$ = 1322
D_x = 1.499 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9899 reflections
θ = 2.2–32.7°
μ = 1.36 mm^{-1}
T = 100 K
Block, clear colourless
0.2 × 0.2 × 0.1 mm

Data collection

Bruker D8 QUEST diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.672, T_{max} = 0.747
230574 measured reflections
11804 independent reflections
10724 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 26.4°, θ_{min} = 2.2°
h = −14→14
k = −14→14
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.066
S = 1.18
11804 reflections
801 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + 7.4732P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 2.69 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data were collected on a Bruker D8 QUEST diffractometer at 100 K, fitted with a CCD area detector employing a mirror-monochromatic Mo $K\alpha$ radiation source (λ = 0.71073 Å). Integration and scaling data of collections were analysed using *APEX3* software. All data was collected with exposures times of 10 s with 1° frame sweeps on ω and φ scans. Multi-scan absorption corrections were used for all compounds. Data was solved in *APEX3* software by intrinsic phasing methods using *SHELXL2019* (Sheldrick, 2015*b*). Refinement of the crystal data was carried out using least-squares refinement methods employed by *SHELXT* (Sheldrick, 2015*a*), with all non-H atoms having anisotropic displacement parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Dy1	0.33364 (2)	0.88334 (2)	0.70770 (2)	0.01421 (4)
O1	0.14213 (18)	0.81836 (17)	0.61567 (9)	0.0226 (4)
O4	0.10417 (16)	0.85927 (16)	0.74764 (9)	0.0184 (4)
O3	0.26817 (17)	0.80274 (16)	0.82902 (9)	0.0180 (4)
O5	0.48381 (17)	0.92885 (17)	0.78364 (9)	0.0211 (4)
O6	0.59713 (19)	0.59441 (19)	0.47168 (10)	0.0288 (5)
N3	0.4241 (2)	1.16415 (19)	0.66016 (10)	0.0165 (4)
N8	0.25145 (19)	0.69586 (18)	0.72208 (10)	0.0154 (4)
N12	0.40730 (19)	0.81566 (18)	0.60874 (10)	0.0149 (4)
N7	0.3101 (2)	0.60256 (19)	0.70496 (11)	0.0168 (5)
N4	0.46876 (19)	1.05553 (19)	0.65707 (10)	0.0159 (4)
N6	0.25488 (19)	1.02076 (18)	0.76828 (10)	0.0152 (4)
N2	0.22899 (19)	1.02888 (18)	0.63156 (10)	0.0147 (4)
N11	0.45877 (19)	0.70935 (19)	0.60896 (11)	0.0159 (4)
N1	0.23337 (19)	1.14425 (19)	0.62994 (10)	0.0158 (4)
O2	0.6523 (2)	0.8894 (2)	0.61141 (12)	0.0454 (6)
N5	0.23727 (19)	1.13627 (19)	0.74612 (10)	0.0160 (4)
N10	0.48552 (19)	0.74328 (19)	0.73665 (10)	0.0172 (5)
N9	0.5089 (2)	0.64199 (19)	0.71726 (11)	0.0185 (5)
C36	0.4310 (2)	0.8765 (2)	0.54694 (12)	0.0167 (5)
H36	0.405174	0.953523	0.532461	0.020*
C37	0.4985 (2)	0.8119 (2)	0.50692 (13)	0.0195 (6)
H37	0.526092	0.834644	0.461366	0.023*
C4	0.1468 (2)	0.9195 (2)	0.56913 (13)	0.0179 (5)
C3	0.1718 (2)	1.0249 (2)	0.58486 (12)	0.0165 (5)
C38	0.5165 (2)	0.7072 (2)	0.54796 (13)	0.0179 (5)
C21	0.2720 (2)	0.6942 (2)	0.87021 (13)	0.0201 (6)
H21	0.301717	0.626055	0.857055	0.024*
C10	0.5867 (2)	1.0671 (2)	0.64575 (13)	0.0192 (6)
C7	0.1187 (3)	0.7326 (3)	0.58867 (15)	0.0250 (6)
H7	0.111585	0.652755	0.609910	0.030*
C12	0.7693 (2)	0.9588 (3)	0.66088 (13)	0.0221 (6)
H12	0.800031	1.007534	0.681469	0.027*
C17	0.2105 (2)	0.9954 (2)	0.83267 (12)	0.0168 (5)
C61	0.7572 (2)	0.1435 (3)	0.91261 (14)	0.0209 (6)
C16	0.1644 (2)	1.0950 (2)	0.85211 (13)	0.0201 (6)
H16	0.128270	1.101652	0.894562	0.024*
C2	0.1429 (2)	1.1360 (2)	0.55333 (13)	0.0210 (6)
H2	0.103708	1.156872	0.518641	0.025*
C22	0.2362 (3)	0.5122 (2)	0.72184 (14)	0.0210 (6)
H22	0.256843	0.437226	0.715240	0.025*
C39	0.5898 (3)	0.6112 (2)	0.53208 (13)	0.0213 (6)
C18	0.2189 (2)	0.8774 (2)	0.86803 (13)	0.0176 (5)
C1	0.1831 (2)	1.2083 (2)	0.58313 (13)	0.0198 (6)
H1	0.176604	1.290233	0.572600	0.024*

C28	0.0128 (2)	0.9335 (3)	0.76307 (13)	0.0217 (6)
H28	0.019545	1.014828	0.756246	0.026*
C15	0.1830 (2)	1.1816 (2)	0.79583 (13)	0.0197 (6)
H15	0.161013	1.260397	0.792641	0.024*
C24	0.1396 (2)	0.6619 (2)	0.74869 (13)	0.0177 (5)
C11	0.6687 (2)	0.9720 (2)	0.64031 (13)	0.0203 (6)
C20	0.2274 (3)	0.7002 (3)	0.93137 (14)	0.0247 (6)
H20	0.220215	0.637740	0.968638	0.030*
C32	0.5506 (2)	0.8369 (3)	0.80790 (13)	0.0210 (6)
C8	0.5121 (3)	1.2384 (2)	0.65158 (14)	0.0226 (6)
H8	0.502933	1.317945	0.651800	0.027*
C25	0.0560 (2)	0.7495 (2)	0.76515 (13)	0.0186 (5)
C5	0.1255 (3)	0.8989 (3)	0.51471 (14)	0.0237 (6)
H5	0.123138	0.954451	0.475528	0.028*
C19	0.1927 (3)	0.8176 (3)	0.93044 (13)	0.0229 (6)
H19	0.157836	0.847529	0.966747	0.027*
C43	0.6039 (3)	0.3058 (2)	0.87102 (14)	0.0231 (6)
C63	0.6815 (3)	−0.0213 (3)	1.00293 (14)	0.0290 (7)
H63	0.620219	−0.053755	1.038602	0.035*
C62	0.6698 (3)	0.0904 (3)	0.96629 (14)	0.0247 (6)
H62	0.600115	0.132522	0.977899	0.030*
C55	0.8084 (3)	0.3667 (3)	0.89706 (13)	0.0236 (6)
C58	0.9376 (3)	0.5266 (3)	0.93217 (15)	0.0363 (8)
H58	0.981343	0.580332	0.942994	0.044*
C9	0.6164 (3)	1.1803 (3)	0.64252 (14)	0.0238 (6)
H9	0.692738	1.210477	0.635522	0.029*
C57	0.9880 (3)	0.4224 (3)	0.92124 (15)	0.0360 (8)
H57	1.066477	0.404005	0.924989	0.043*
C66	0.8576 (3)	0.0757 (3)	0.90002 (14)	0.0269 (6)
H66	0.919972	0.107600	0.864836	0.032*
C44	0.5526 (3)	0.2958 (2)	0.82047 (15)	0.0246 (6)
H44	0.600744	0.271918	0.784681	0.029*
C23	0.1267 (3)	0.5454 (2)	0.75002 (14)	0.0227 (6)
H23	0.057776	0.499803	0.766661	0.027*
C31	0.5541 (2)	0.7413 (2)	0.77859 (13)	0.0197 (6)
C27	−0.0867 (3)	0.8735 (3)	0.78908 (14)	0.0257 (6)
H27	−0.161641	0.904253	0.804011	0.031*
C6	0.1074 (3)	0.7781 (3)	0.52786 (15)	0.0274 (7)
H6	0.090519	0.737058	0.499017	0.033*
C60	0.7601 (3)	0.4715 (3)	0.90957 (14)	0.0274 (7)
H60	0.681495	0.489812	0.906070	0.033*
C26	−0.0598 (2)	0.7550 (3)	0.79034 (14)	0.0246 (6)
H26	−0.113186	0.692161	0.805910	0.029*
C65	0.8710 (3)	−0.0360 (3)	0.93631 (15)	0.0313 (7)
H65	0.941263	−0.077993	0.925725	0.038*
C35	0.4949 (3)	1.0148 (3)	0.81415 (15)	0.0271 (7)
H35	0.458912	1.089008	0.806521	0.033*
C29	0.5899 (3)	0.5799 (2)	0.74667 (14)	0.0245 (6)

H29	0.620159	0.506547	0.741143	0.029*
C45	0.4347 (3)	0.3192 (3)	0.82047 (18)	0.0332 (7)
H45	0.403936	0.310474	0.785409	0.040*
B1	0.2915 (3)	1.1922 (3)	0.67439 (14)	0.0161 (6)
C54	0.8456 (2)	0.4054 (3)	0.75453 (14)	0.0231 (6)
H54	0.833191	0.467997	0.774922	0.028*
C40	0.6622 (3)	0.5371 (3)	0.56241 (15)	0.0319 (7)
H40	0.675304	0.532156	0.604194	0.038*
C33	0.5994 (3)	0.8626 (3)	0.85277 (14)	0.0289 (7)
H33	0.648000	0.813458	0.877412	0.035*
C64	0.7821 (3)	−0.0858 (3)	0.98776 (15)	0.0303 (7)
H64	0.789737	−0.162573	1.012233	0.036*
C42	0.6748 (3)	0.5052 (3)	0.46568 (18)	0.0358 (8)
H42	0.696777	0.474617	0.428517	0.043*
C30	0.6211 (3)	0.6405 (3)	0.78584 (15)	0.0264 (6)
H30	0.676584	0.618376	0.812241	0.032*
C56	0.9226 (3)	0.3457 (3)	0.90482 (14)	0.0289 (7)
H56	0.958300	0.274607	0.898537	0.035*
C59	0.8229 (3)	0.5499 (3)	0.92693 (15)	0.0343 (8)
H59	0.786465	0.619573	0.935173	0.041*
C52	0.9183 (3)	0.3394 (3)	0.65763 (15)	0.0299 (7)
H52	0.954349	0.354105	0.612910	0.036*
C41	0.7151 (3)	0.4675 (3)	0.51901 (18)	0.0385 (9)
H41	0.769065	0.405727	0.526885	0.046*
C49	0.8126 (2)	0.2947 (3)	0.79244 (14)	0.0214 (6)
C51	0.8878 (3)	0.2281 (3)	0.69290 (15)	0.0301 (7)
H51	0.903250	0.165655	0.672410	0.036*
B2	0.4413 (3)	0.6116 (3)	0.67174 (15)	0.0175 (6)
C53	0.8956 (3)	0.4291 (3)	0.68858 (15)	0.0298 (7)
H53	0.914021	0.506421	0.664894	0.036*
C46	0.3628 (3)	0.3549 (3)	0.87126 (19)	0.0386 (8)
H46	0.282786	0.372963	0.870982	0.046*
C34	0.5641 (3)	0.9775 (3)	0.85608 (16)	0.0343 (8)
H34	0.585650	1.019889	0.883051	0.041*
B3	0.7436 (3)	0.2764 (3)	0.86923 (16)	0.0213 (6)
C50	0.8342 (3)	0.2070 (3)	0.75859 (14)	0.0254 (6)
H50	0.811336	0.130178	0.781337	0.030*
C48	0.5260 (3)	0.3384 (3)	0.92266 (17)	0.0344 (7)
H48	0.554376	0.343198	0.959207	0.041*
C14	0.7504 (5)	0.8162 (3)	0.61536 (18)	0.0587 (14)
H14	0.764460	0.748716	0.599164	0.070*
C47	0.4077 (3)	0.3641 (3)	0.92232 (19)	0.0426 (9)
H47	0.358356	0.388041	0.957725	0.051*
C13	0.8197 (4)	0.8552 (4)	0.64484 (18)	0.0548 (13)
H13	0.891004	0.820380	0.653869	0.066*
H1A	0.277 (3)	1.284 (3)	0.6654 (14)	0.015 (7)*
H2A	0.473 (2)	0.529 (2)	0.6616 (13)	0.009 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Dy1	0.01689 (6)	0.01315 (6)	0.01179 (6)	−0.00031 (4)	−0.00197 (4)	−0.00260 (4)
O1	0.0278 (11)	0.0197 (10)	0.0212 (10)	0.0018 (8)	−0.0080 (8)	−0.0047 (8)
O4	0.0192 (9)	0.0163 (9)	0.0194 (10)	−0.0006 (7)	−0.0024 (8)	−0.0056 (8)
O3	0.0236 (10)	0.0161 (9)	0.0122 (9)	−0.0011 (7)	−0.0021 (7)	−0.0012 (7)
O5	0.0247 (10)	0.0207 (10)	0.0182 (10)	−0.0029 (8)	−0.0050 (8)	−0.0041 (8)
O6	0.0337 (12)	0.0281 (11)	0.0238 (11)	0.0023 (9)	0.0007 (9)	−0.0119 (9)
N3	0.0197 (11)	0.0151 (11)	0.0139 (11)	−0.0021 (9)	−0.0011 (9)	−0.0039 (9)
N8	0.0183 (11)	0.0139 (11)	0.0129 (10)	−0.0006 (8)	−0.0019 (9)	−0.0026 (8)
N12	0.0176 (11)	0.0116 (10)	0.0148 (11)	0.0016 (8)	−0.0024 (9)	−0.0034 (8)
N7	0.0218 (12)	0.0134 (11)	0.0151 (11)	−0.0009 (9)	−0.0027 (9)	−0.0044 (9)
N4	0.0183 (11)	0.0171 (11)	0.0122 (10)	−0.0004 (9)	−0.0028 (9)	−0.0038 (9)
N6	0.0186 (11)	0.0132 (10)	0.0129 (10)	−0.0011 (8)	−0.0022 (9)	−0.0027 (8)
N2	0.0173 (11)	0.0135 (10)	0.0129 (10)	−0.0004 (8)	−0.0017 (8)	−0.0038 (8)
N11	0.0173 (11)	0.0140 (11)	0.0151 (11)	0.0018 (8)	−0.0004 (9)	−0.0044 (9)
N1	0.0174 (11)	0.0137 (11)	0.0155 (11)	0.0001 (8)	−0.0024 (9)	−0.0032 (9)
O2	0.0546 (17)	0.0431 (15)	0.0383 (14)	−0.0146 (13)	−0.0060 (12)	−0.0102 (12)
N5	0.0183 (11)	0.0150 (11)	0.0142 (11)	−0.0019 (9)	−0.0017 (9)	−0.0040 (9)
N10	0.0187 (11)	0.0182 (11)	0.0134 (11)	0.0003 (9)	−0.0021 (9)	−0.0029 (9)
N9	0.0207 (12)	0.0147 (11)	0.0174 (11)	0.0009 (9)	−0.0029 (9)	−0.0002 (9)
C36	0.0200 (13)	0.0153 (13)	0.0135 (12)	0.0011 (10)	−0.0030 (10)	−0.0021 (10)
C37	0.0226 (14)	0.0214 (14)	0.0134 (13)	0.0017 (11)	−0.0015 (11)	−0.0051 (11)
C4	0.0162 (13)	0.0209 (14)	0.0164 (13)	0.0003 (10)	−0.0049 (10)	−0.0030 (11)
C3	0.0134 (12)	0.0227 (14)	0.0130 (12)	0.0013 (10)	−0.0007 (10)	−0.0057 (10)
C38	0.0178 (13)	0.0195 (13)	0.0177 (13)	0.0015 (10)	−0.0030 (10)	−0.0080 (11)
C21	0.0240 (14)	0.0147 (13)	0.0193 (14)	−0.0033 (11)	−0.0067 (11)	0.0027 (11)
C10	0.0180 (13)	0.0250 (14)	0.0135 (12)	−0.0024 (11)	−0.0031 (10)	−0.0025 (11)
C7	0.0255 (15)	0.0199 (14)	0.0341 (17)	0.0016 (11)	−0.0111 (13)	−0.0111 (13)
C12	0.0158 (13)	0.0371 (17)	0.0175 (13)	0.0053 (12)	−0.0082 (11)	−0.0112 (12)
C17	0.0175 (13)	0.0210 (14)	0.0134 (12)	−0.0028 (10)	−0.0032 (10)	−0.0065 (10)
C61	0.0184 (13)	0.0257 (15)	0.0202 (14)	−0.0038 (11)	−0.0066 (11)	−0.0055 (12)
C16	0.0207 (14)	0.0246 (14)	0.0161 (13)	−0.0026 (11)	−0.0004 (11)	−0.0099 (11)
C2	0.0203 (14)	0.0243 (15)	0.0187 (14)	0.0025 (11)	−0.0085 (11)	−0.0022 (11)
C22	0.0275 (15)	0.0125 (13)	0.0229 (14)	−0.0025 (11)	−0.0060 (12)	−0.0034 (11)
C39	0.0261 (15)	0.0174 (13)	0.0179 (13)	−0.0009 (11)	0.0022 (11)	−0.0060 (11)
C18	0.0174 (13)	0.0215 (14)	0.0147 (13)	−0.0018 (10)	−0.0028 (10)	−0.0062 (11)
C1	0.0200 (13)	0.0174 (13)	0.0188 (13)	0.0039 (10)	−0.0037 (11)	−0.0002 (11)
C28	0.0216 (14)	0.0239 (14)	0.0207 (14)	0.0057 (11)	−0.0048 (11)	−0.0087 (12)
C15	0.0210 (14)	0.0178 (13)	0.0209 (14)	−0.0012 (11)	−0.0001 (11)	−0.0096 (11)
C24	0.0175 (13)	0.0204 (14)	0.0144 (12)	−0.0043 (10)	−0.0039 (10)	−0.0012 (10)
C11	0.0192 (13)	0.0232 (14)	0.0160 (13)	−0.0051 (11)	−0.0019 (11)	−0.0005 (11)
C20	0.0280 (15)	0.0273 (15)	0.0151 (13)	−0.0057 (12)	−0.0043 (11)	0.0025 (12)
C32	0.0183 (13)	0.0268 (15)	0.0153 (13)	−0.0026 (11)	−0.0040 (11)	0.0008 (11)
C8	0.0261 (15)	0.0186 (14)	0.0220 (14)	−0.0081 (11)	−0.0008 (12)	−0.0050 (11)
C25	0.0206 (14)	0.0197 (13)	0.0137 (13)	−0.0047 (11)	−0.0026 (10)	−0.0009 (10)
C5	0.0238 (15)	0.0287 (16)	0.0207 (14)	0.0048 (12)	−0.0088 (12)	−0.0076 (12)

C19	0.0260 (15)	0.0284 (15)	0.0128 (13)	−0.0040 (12)	−0.0024 (11)	−0.0034 (11)
C43	0.0232 (14)	0.0168 (14)	0.0255 (15)	−0.0017 (11)	−0.0016 (12)	−0.0014 (11)
C63	0.0326 (17)	0.0356 (17)	0.0180 (14)	−0.0099 (14)	−0.0041 (12)	−0.0038 (13)
C62	0.0249 (15)	0.0303 (16)	0.0212 (14)	−0.0032 (12)	−0.0052 (12)	−0.0096 (12)
C55	0.0287 (15)	0.0285 (15)	0.0108 (12)	−0.0093 (12)	−0.0007 (11)	−0.0004 (11)
C58	0.055 (2)	0.0363 (19)	0.0169 (15)	−0.0252 (16)	−0.0060 (14)	−0.0009 (13)
C9	0.0211 (14)	0.0242 (15)	0.0255 (15)	−0.0073 (11)	−0.0042 (12)	−0.0040 (12)
C57	0.0284 (17)	0.058 (2)	0.0198 (15)	−0.0171 (16)	−0.0015 (13)	−0.0046 (15)
C66	0.0252 (15)	0.0318 (17)	0.0208 (15)	−0.0008 (12)	−0.0028 (12)	−0.0031 (12)
C44	0.0203 (14)	0.0192 (14)	0.0320 (16)	−0.0026 (11)	−0.0046 (12)	−0.0026 (12)
C23	0.0268 (15)	0.0178 (14)	0.0223 (14)	−0.0077 (11)	−0.0038 (12)	−0.0022 (11)
C31	0.0186 (13)	0.0241 (14)	0.0129 (12)	−0.0041 (11)	−0.0039 (10)	0.0032 (11)
C27	0.0182 (14)	0.0331 (17)	0.0246 (15)	0.0024 (12)	−0.0015 (12)	−0.0081 (13)
C6	0.0282 (16)	0.0295 (16)	0.0331 (17)	0.0078 (13)	−0.0155 (13)	−0.0177 (14)
C60	0.0381 (18)	0.0256 (15)	0.0156 (14)	−0.0040 (13)	−0.0072 (12)	0.0025 (12)
C26	0.0176 (14)	0.0301 (16)	0.0223 (15)	−0.0050 (12)	−0.0026 (11)	0.0000 (12)
C65	0.0346 (18)	0.0322 (17)	0.0257 (16)	0.0048 (14)	−0.0078 (13)	−0.0049 (13)
C35	0.0281 (16)	0.0272 (16)	0.0282 (16)	−0.0076 (12)	−0.0014 (13)	−0.0132 (13)
C29	0.0231 (14)	0.0174 (14)	0.0286 (16)	0.0036 (11)	−0.0067 (12)	0.0025 (12)
C45	0.0234 (16)	0.0259 (16)	0.048 (2)	−0.0017 (13)	−0.0098 (14)	−0.0026 (15)
B1	0.0172 (14)	0.0148 (14)	0.0149 (14)	−0.0015 (11)	−0.0016 (11)	−0.0026 (11)
C54	0.0210 (14)	0.0273 (15)	0.0223 (14)	0.0003 (11)	−0.0061 (11)	−0.0072 (12)
C40	0.0298 (17)	0.0397 (19)	0.0216 (15)	0.0095 (14)	−0.0023 (13)	−0.0040 (14)
C33	0.0231 (15)	0.0450 (19)	0.0197 (15)	−0.0036 (13)	−0.0079 (12)	−0.0061 (13)
C64	0.0440 (19)	0.0250 (16)	0.0222 (15)	−0.0037 (14)	−0.0123 (14)	−0.0011 (12)
C42	0.0378 (19)	0.0246 (16)	0.042 (2)	0.0013 (14)	0.0090 (15)	−0.0192 (15)
C30	0.0230 (15)	0.0248 (15)	0.0294 (16)	0.0011 (12)	−0.0130 (12)	0.0036 (12)
C56	0.0164 (14)	0.049 (2)	0.0189 (14)	−0.0096 (13)	0.0078 (11)	−0.0114 (14)
C59	0.061 (2)	0.0230 (16)	0.0179 (15)	−0.0095 (15)	−0.0101 (15)	0.0016 (12)
C52	0.0222 (15)	0.049 (2)	0.0176 (14)	−0.0004 (14)	−0.0012 (12)	−0.0084 (14)
C41	0.0366 (19)	0.0213 (16)	0.043 (2)	0.0081 (14)	0.0099 (16)	0.0003 (14)
C49	0.0166 (13)	0.0285 (15)	0.0200 (14)	0.0000 (11)	−0.0055 (11)	−0.0062 (12)
C51	0.0329 (17)	0.0364 (18)	0.0252 (16)	0.0058 (14)	−0.0090 (13)	−0.0143 (14)
B2	0.0185 (15)	0.0151 (14)	0.0161 (14)	−0.0007 (11)	−0.0006 (12)	−0.0015 (12)
C53	0.0283 (16)	0.0355 (18)	0.0230 (15)	−0.0054 (13)	−0.0036 (13)	−0.0026 (13)
C46	0.0184 (15)	0.0313 (18)	0.060 (2)	0.0009 (13)	−0.0014 (15)	−0.0059 (17)
C34	0.0282 (17)	0.052 (2)	0.0278 (17)	−0.0130 (15)	−0.0042 (13)	−0.0171 (15)
B3	0.0199 (15)	0.0248 (16)	0.0193 (15)	−0.0014 (12)	−0.0023 (12)	−0.0068 (13)
C50	0.0260 (15)	0.0262 (15)	0.0240 (15)	−0.0003 (12)	−0.0074 (12)	−0.0046 (12)
C48	0.0294 (17)	0.0351 (18)	0.0348 (18)	−0.0029 (14)	0.0025 (14)	−0.0092 (15)
C14	0.111 (4)	0.0245 (19)	0.0262 (19)	0.008 (2)	0.010 (2)	−0.0058 (15)
C47	0.0308 (18)	0.038 (2)	0.049 (2)	0.0019 (15)	0.0109 (16)	−0.0128 (17)
C13	0.041 (2)	0.076 (3)	0.0274 (19)	0.039 (2)	0.0006 (16)	0.0085 (19)

Geometric parameters (Å, º)

Dy1—O4	2.6400 (19)	C20—H20	0.9500
Dy1—O3	2.5419 (18)	C20—C19	1.432 (4)

Dy1—O5	2.8418 (19)	C32—C31	1.437 (4)
Dy1—N8	2.411 (2)	C32—C33	1.349 (4)
Dy1—N12	2.455 (2)	C8—H8	0.9500
Dy1—N4	2.534 (2)	C8—C9	1.367 (4)
Dy1—N6	2.375 (2)	C25—C26	1.347 (4)
Dy1—N2	2.558 (2)	C5—H5	0.9500
Dy1—N10	2.448 (2)	C5—C6	1.419 (4)
O1—C4	1.367 (3)	C19—H19	0.9500
O1—C7	1.373 (3)	C43—C44	1.409 (4)
O4—C28	1.384 (3)	C43—B3	1.647 (4)
O4—C25	1.387 (3)	C43—C48	1.402 (4)
O3—C21	1.387 (3)	C63—H63	0.9500
O3—C18	1.396 (3)	C63—C62	1.392 (4)
O5—C32	1.377 (3)	C63—C64	1.389 (5)
O5—C35	1.384 (3)	C62—H62	0.9500
O6—C39	1.370 (3)	C55—C60	1.404 (4)
O6—C42	1.370 (4)	C55—C56	1.388 (4)
N3—N4	1.380 (3)	C55—B3	1.659 (4)
N3—C8	1.351 (3)	C58—H58	0.9500
N3—B1	1.545 (4)	C58—C57	1.395 (5)
N8—N7	1.360 (3)	C58—C59	1.382 (5)
N8—C24	1.349 (3)	C9—H9	0.9500
N12—N11	1.371 (3)	C57—H57	0.9500
N12—C36	1.342 (3)	C57—C56	1.390 (5)
N7—C22	1.349 (3)	C66—H66	0.9500
N7—B2	1.540 (4)	C66—C65	1.392 (4)
N4—C10	1.356 (3)	C44—H44	0.9500
N6—N5	1.363 (3)	C44—C45	1.394 (4)
N6—C17	1.350 (3)	C23—H23	0.9500
N2—N1	1.373 (3)	C31—C30	1.392 (4)
N2—C3	1.357 (3)	C27—H27	0.9500
N11—C38	1.358 (3)	C27—C26	1.425 (4)
N11—B2	1.548 (4)	C6—H6	0.9500
N1—C1	1.348 (3)	C60—H60	0.9500
N1—B1	1.540 (4)	C60—C59	1.398 (4)
O2—C11	1.342 (4)	C26—H26	0.9500
O2—C14	1.406 (5)	C65—H65	0.9500
N5—C15	1.348 (3)	C65—C64	1.383 (5)
N5—B1	1.546 (4)	C35—H35	0.9500
N10—N9	1.371 (3)	C35—C34	1.340 (5)
N10—C31	1.348 (3)	C29—H29	0.9500
N9—C29	1.350 (4)	C29—C30	1.371 (4)
N9—B2	1.527 (4)	C45—H45	0.9500
C36—H36	0.9500	C45—C46	1.375 (5)
C36—C37	1.390 (4)	B1—H1A	1.07 (3)
C37—H37	0.9500	C54—H54	0.9500
C37—C38	1.382 (4)	C54—C49	1.399 (4)
C4—C3	1.449 (4)	C54—C53	1.393 (4)

C4—C5	1.354 (4)	C40—H40	0.9500
C3—C2	1.396 (4)	C40—C41	1.428 (5)
C38—C39	1.454 (4)	C33—H33	0.9500
C21—H21	0.9500	C33—C34	1.423 (5)
C21—C20	1.340 (4)	C64—H64	0.9500
C10—C11	1.452 (4)	C42—H42	0.9500
C10—C9	1.398 (4)	C42—C41	1.325 (5)
C7—H7	0.9500	C30—H30	0.9500
C7—C6	1.342 (4)	C56—H56	0.9500
C12—H12	0.9500	C59—H59	0.9500
C12—C11	1.343 (4)	C52—H52	0.9500
C12—C13	1.426 (5)	C52—C51	1.382 (5)
C17—C16	1.398 (4)	C52—C53	1.387 (5)
C17—C18	1.438 (4)	C41—H41	0.9500
C61—C62	1.410 (4)	C49—B3	1.657 (4)
C61—C66	1.401 (4)	C49—C50	1.406 (4)
C61—B3	1.653 (4)	C51—H51	0.9500
C16—H16	0.9500	C51—C50	1.398 (4)
C16—C15	1.380 (4)	B2—H2A	1.09 (3)
C2—H2	0.9500	C53—H53	0.9500
C2—C1	1.365 (4)	C46—H46	0.9500
C22—H22	0.9500	C46—C47	1.371 (6)
C22—C23	1.372 (4)	C34—H34	0.9500
C39—C40	1.348 (4)	C50—H50	0.9500
C18—C19	1.350 (4)	C48—H48	0.9500
C1—H1	0.9500	C48—C47	1.403 (5)
C28—H28	0.9500	C14—H14	0.9500
C28—C27	1.338 (4)	C14—C13	1.316 (7)
C15—H15	0.9500	C47—H47	0.9500
C24—C25	1.444 (4)	C13—H13	0.9500
C24—C23	1.400 (4)		

O4—Dy1—O5	124.32 (6)	O5—C32—C31	113.8 (2)
O3—Dy1—O4	66.82 (6)	C33—C32—O5	109.8 (3)
O3—Dy1—O5	64.03 (6)	C33—C32—C31	136.3 (3)
O3—Dy1—N2	128.88 (6)	N3—C8—H8	125.6
N8—Dy1—O4	61.90 (7)	N3—C8—C9	108.8 (3)
N8—Dy1—O3	73.97 (7)	C9—C8—H8	125.6
N8—Dy1—O5	123.56 (6)	O4—C25—C24	113.2 (2)
N8—Dy1—N12	71.16 (7)	C26—C25—O4	109.9 (2)
N8—Dy1—N4	158.30 (7)	C26—C25—C24	136.8 (3)
N8—Dy1—N2	107.17 (7)	C4—C5—H5	126.8
N8—Dy1—N10	74.41 (7)	C4—C5—C6	106.3 (3)
N12—Dy1—O4	111.51 (7)	C6—C5—H5	126.8
N12—Dy1—O3	139.83 (6)	C18—C19—C20	106.8 (3)
N12—Dy1—O5	122.63 (7)	C18—C19—H19	126.6
N12—Dy1—N4	87.73 (7)	C20—C19—H19	126.6
N12—Dy1—N2	80.96 (7)	C44—C43—B3	121.5 (3)

N4—Dy1—O4	134.12 (6)	C48—C43—C44	114.7 (3)
N4—Dy1—O3	123.38 (6)	C48—C43—B3	123.8 (3)
N4—Dy1—O5	63.69 (6)	C62—C63—H63	119.7
N4—Dy1—N2	73.26 (7)	C64—C63—H63	119.7
N6—Dy1—O4	69.71 (7)	C64—C63—C62	120.5 (3)
N6—Dy1—O3	64.43 (7)	C61—C62—H62	118.7
N6—Dy1—O5	66.74 (7)	C63—C62—C61	122.6 (3)
N6—Dy1—N8	125.28 (7)	C63—C62—H62	118.7
N6—Dy1—N12	155.31 (7)	C60—C55—B3	125.1 (3)
N6—Dy1—N4	76.30 (7)	C56—C55—C60	114.7 (3)
N6—Dy1—N2	76.50 (7)	C56—C55—B3	120.0 (3)
N6—Dy1—N10	122.87 (7)	C57—C58—H58	120.7
N2—Dy1—O4	69.58 (6)	C59—C58—H58	120.7
N2—Dy1—O5	128.19 (6)	C59—C58—C57	118.6 (3)
N10—Dy1—O4	127.69 (7)	C10—C9—H9	127.4
N10—Dy1—O3	74.91 (7)	C8—C9—C10	105.2 (2)
N10—Dy1—O5	59.90 (7)	C8—C9—H9	127.4
N10—Dy1—N12	77.02 (7)	C58—C57—H57	120.2
N10—Dy1—N4	96.45 (7)	C56—C57—C58	119.6 (3)
N10—Dy1—N2	156.07 (7)	C56—C57—H57	120.2
C4—O1—C7	106.5 (2)	C61—C66—H66	118.2
C28—O4—Dy1	134.04 (17)	C65—C66—C61	123.5 (3)
C28—O4—C25	106.2 (2)	C65—C66—H66	118.2
C25—O4—Dy1	119.33 (16)	C43—C44—H44	118.4
C21—O3—Dy1	134.34 (16)	C45—C44—C43	123.1 (3)
C21—O3—C18	106.4 (2)	C45—C44—H44	118.4
C18—O3—Dy1	119.20 (15)	C22—C23—C24	104.3 (2)
C32—O5—Dy1	115.82 (16)	C22—C23—H23	127.8
C32—O5—C35	106.5 (2)	C24—C23—H23	127.8
C35—O5—Dy1	136.43 (18)	N10—C31—C32	119.5 (2)
C39—O6—C42	106.3 (3)	N10—C31—C30	110.7 (3)
N4—N3—B1	123.5 (2)	C30—C31—C32	129.7 (3)
C8—N3—N4	110.2 (2)	C28—C27—H27	126.2
C8—N3—B1	126.2 (2)	C28—C27—C26	107.7 (3)
N7—N8—Dy1	126.24 (16)	C26—C27—H27	126.2
C24—N8—Dy1	127.46 (18)	C7—C6—C5	107.2 (3)
C24—N8—N7	106.3 (2)	C7—C6—H6	126.4
N11—N12—Dy1	122.81 (16)	C5—C6—H6	126.4
C36—N12—Dy1	129.32 (17)	C55—C60—H60	118.6
C36—N12—N11	106.2 (2)	C59—C60—C55	122.8 (3)
N8—N7—B2	120.2 (2)	C59—C60—H60	118.6
C22—N7—N8	109.5 (2)	C25—C26—C27	106.6 (3)
C22—N7—B2	130.3 (2)	C25—C26—H26	126.7
N3—N4—Dy1	118.27 (15)	C27—C26—H26	126.7
C10—N4—Dy1	132.64 (18)	C66—C65—H65	120.0
C10—N4—N3	104.9 (2)	C64—C65—C66	120.0 (3)
N5—N6—Dy1	128.32 (16)	C64—C65—H65	120.0
C17—N6—Dy1	125.03 (17)	O5—C35—H35	125.2

C17—N6—N5	106.5 (2)	C34—C35—O5	109.6 (3)
N1—N2—Dy1	118.84 (15)	C34—C35—H35	125.2
C3—N2—Dy1	136.12 (17)	N9—C29—H29	125.7
C3—N2—N1	104.8 (2)	N9—C29—C30	108.6 (3)
N12—N11—B2	120.9 (2)	C30—C29—H29	125.7
C38—N11—N12	109.4 (2)	C44—C45—H45	120.0
C38—N11—B2	129.6 (2)	C46—C45—C44	120.0 (3)
N2—N1—B1	124.0 (2)	C46—C45—H45	120.0
C1—N1—N2	110.4 (2)	N3—B1—N5	109.0 (2)
C1—N1—B1	125.5 (2)	N3—B1—H1A	110.5 (16)
C11—O2—C14	104.5 (3)	N1—B1—N3	109.1 (2)
N6—N5—B1	117.7 (2)	N1—B1—N5	110.4 (2)
C15—N5—N6	109.6 (2)	N1—B1—H1A	108.7 (16)
C15—N5—B1	132.3 (2)	N5—B1—H1A	109.1 (16)
N9—N10—Dy1	125.14 (16)	C49—C54—H54	118.1
C31—N10—Dy1	128.95 (18)	C53—C54—H54	118.1
C31—N10—N9	105.6 (2)	C53—C54—C49	123.7 (3)
N10—N9—B2	120.1 (2)	C39—C40—H40	127.0
C29—N9—N10	110.0 (2)	C39—C40—C41	106.1 (3)
C29—N9—B2	129.8 (2)	C41—C40—H40	127.0
N12—C36—H36	124.5	C32—C33—H33	126.6
N12—C36—C37	111.0 (2)	C32—C33—C34	106.8 (3)
C37—C36—H36	124.5	C34—C33—H33	126.6
C36—C37—H37	127.6	C63—C64—H64	120.7
C38—C37—C36	104.9 (2)	C65—C64—C63	118.6 (3)
C38—C37—H37	127.6	C65—C64—H64	120.7
O1—C4—C3	118.0 (2)	O6—C42—H42	124.8
C5—C4—O1	110.1 (2)	C41—C42—O6	110.5 (3)
C5—C4—C3	132.0 (3)	C41—C42—H42	124.8
N2—C3—C4	124.3 (2)	C31—C30—H30	127.4
N2—C3—C2	110.9 (2)	C29—C30—C31	105.1 (3)
C2—C3—C4	124.8 (2)	C29—C30—H30	127.4
N11—C38—C37	108.4 (2)	C55—C56—C57	124.0 (3)
N11—C38—C39	123.6 (2)	C55—C56—H56	118.0
C37—C38—C39	127.8 (2)	C57—C56—H56	118.0
O3—C21—H21	125.2	C58—C59—C60	120.3 (3)
C20—C21—O3	109.7 (3)	C58—C59—H59	119.8
C20—C21—H21	125.2	C60—C59—H59	119.8
N4—C10—C11	123.5 (2)	C51—C52—H52	120.5
N4—C10—C9	110.9 (2)	C51—C52—C53	118.9 (3)
C9—C10—C11	125.6 (3)	C53—C52—H52	120.5
O1—C7—H7	125.0	C40—C41—H41	126.4
C6—C7—O1	110.0 (3)	C42—C41—C40	107.1 (3)
C6—C7—H7	125.0	C42—C41—H41	126.4
C11—C12—H12	127.8	C54—C49—B3	120.2 (3)
C11—C12—C13	104.5 (3)	C54—C49—C50	114.5 (3)
C13—C12—H12	127.8	C50—C49—B3	125.1 (3)
N6—C17—C16	110.3 (2)	C52—C51—H51	119.9

N6—C17—C18	117.5 (2)	C52—C51—C50	120.3 (3)
C16—C17—C18	132.2 (2)	C50—C51—H51	119.9
C62—C61—B3	122.7 (3)	N7—B2—N11	109.2 (2)
C66—C61—C62	114.6 (3)	N7—B2—H2A	109.7 (15)
C66—C61—B3	122.7 (3)	N11—B2—H2A	111.2 (14)
C17—C16—H16	127.7	N9—B2—N7	108.6 (2)
C15—C16—C17	104.6 (2)	N9—B2—N11	108.9 (2)
C15—C16—H16	127.7	N9—B2—H2A	109.2 (14)
C3—C2—H2	127.5	C54—C53—H53	120.1
C1—C2—C3	105.1 (2)	C52—C53—C54	119.7 (3)
C1—C2—H2	127.5	C52—C53—H53	120.1
N7—C22—H22	125.3	C45—C46—H46	120.3
N7—C22—C23	109.4 (2)	C47—C46—C45	119.3 (3)
C23—C22—H22	125.3	C47—C46—H46	120.3
O6—C39—C38	116.0 (2)	C35—C34—C33	107.4 (3)
C40—C39—O6	110.0 (3)	C35—C34—H34	126.3
C40—C39—C38	133.7 (3)	C33—C34—H34	126.3
O3—C18—C17	113.7 (2)	C61—B3—C55	108.5 (2)
C19—C18—O3	109.4 (2)	C61—B3—C49	112.8 (2)
C19—C18—C17	136.9 (3)	C43—B3—C61	109.4 (2)
N1—C1—C2	108.8 (2)	C43—B3—C55	113.5 (2)
N1—C1—H1	125.6	C43—B3—C49	107.5 (2)
C2—C1—H1	125.6	C49—B3—C55	105.0 (2)
O4—C28—H28	125.2	C49—C50—H50	118.6
C27—C28—O4	109.7 (3)	C51—C50—C49	122.8 (3)
C27—C28—H28	125.2	C51—C50—H50	118.6
N5—C15—C16	109.1 (2)	C43—C48—H48	118.8
N5—C15—H15	125.5	C43—C48—C47	122.4 (3)
C16—C15—H15	125.5	C47—C48—H48	118.8
N8—C24—C25	117.1 (2)	O2—C14—H14	125.1
N8—C24—C23	110.5 (2)	C13—C14—O2	109.9 (3)
C23—C24—C25	132.3 (3)	C13—C14—H14	125.1
O2—C11—C10	122.2 (3)	C46—C47—C48	120.5 (3)
O2—C11—C12	113.0 (3)	C46—C47—H47	119.7
C12—C11—C10	124.8 (3)	C48—C47—H47	119.7
C21—C20—H20	126.2	C12—C13—H13	125.9
C21—C20—C19	107.7 (3)	C14—C13—C12	108.2 (3)
C19—C20—H20	126.2	C14—C13—H13	125.9

Dy1—O4—C28—C27	−171.86 (18)	C61—C66—C65—C64	0.3 (5)
Dy1—O4—C25—C24	−9.7 (3)	C16—C17—C18—O3	177.6 (3)
Dy1—O4—C25—C26	173.52 (18)	C16—C17—C18—C19	−3.4 (6)
Dy1—O3—C21—C20	178.26 (18)	C22—N7—B2—N11	122.5 (3)
Dy1—O3—C18—C17	0.4 (3)	C22—N7—B2—N9	−118.9 (3)
Dy1—O3—C18—C19	−178.83 (18)	C39—O6—C42—C41	−0.2 (4)
Dy1—O5—C32—C31	13.9 (3)	C39—C40—C41—C42	1.7 (4)
Dy1—O5—C32—C33	−167.88 (19)	C18—O3—C21—C20	0.2 (3)
Dy1—O5—C35—C34	165.1 (2)	C18—C17—C16—C15	179.7 (3)

Dy1—N8—N7—C22	178.53 (17)	C1—N1—B1—N3	−114.7 (3)
Dy1—N8—N7—B2	−1.3 (3)	C1—N1—B1—N5	125.5 (3)
Dy1—N8—C24—C25	6.4 (3)	C28—O4—C25—C24	176.7 (2)
Dy1—N8—C24—C23	−178.35 (18)	C28—O4—C25—C26	0.0 (3)
Dy1—N12—N11—C38	−164.64 (17)	C28—C27—C26—C25	0.4 (3)
Dy1—N12—N11—B2	18.4 (3)	C15—N5—B1—N3	118.1 (3)
Dy1—N12—C36—C37	164.70 (18)	C15—N5—B1—N1	−122.1 (3)
Dy1—N4—C10—C11	22.9 (4)	C24—N8—N7—C22	−1.1 (3)
Dy1—N4—C10—C9	−154.99 (19)	C24—N8—N7—B2	179.0 (2)
Dy1—N6—N5—C15	175.58 (18)	C24—C25—C26—C27	−175.8 (3)
Dy1—N6—N5—B1	−10.7 (3)	C11—O2—C14—C13	−0.2 (4)
Dy1—N6—C17—C16	−175.93 (17)	C11—C10—C9—C8	−178.5 (3)
Dy1—N6—C17—C18	4.5 (3)	C11—C12—C13—C14	1.6 (4)
Dy1—N2—N1—C1	174.34 (16)	C32—O5—C35—C34	−0.8 (3)
Dy1—N2—N1—B1	−3.9 (3)	C32—C31—C30—C29	−179.8 (3)
Dy1—N2—C3—C4	5.6 (4)	C32—C33—C34—C35	0.9 (4)
Dy1—N2—C3—C2	−173.16 (18)	C8—N3—N4—Dy1	159.39 (17)
Dy1—N10—N9—C29	−174.11 (18)	C8—N3—N4—C10	−0.5 (3)
Dy1—N10—N9—B2	2.7 (3)	C8—N3—B1—N1	133.3 (3)
Dy1—N10—C31—C32	−6.6 (4)	C8—N3—B1—N5	−106.0 (3)
Dy1—N10—C31—C30	174.06 (18)	C25—O4—C28—C27	0.3 (3)
O1—C4—C3—N2	23.6 (4)	C25—C24—C23—C22	173.3 (3)
O1—C4—C3—C2	−157.9 (3)	C5—C4—C3—N2	−156.6 (3)
O1—C4—C5—C6	−0.5 (3)	C5—C4—C3—C2	22.0 (5)
O1—C7—C6—C5	0.6 (3)	C43—C44—C45—C46	0.6 (5)
O4—C28—C27—C26	−0.5 (3)	C43—C48—C47—C46	1.9 (5)
O4—C25—C26—C27	−0.2 (3)	C62—C61—C66—C65	1.0 (4)
O3—C21—C20—C19	0.1 (3)	C62—C61—B3—C43	−29.5 (4)
O3—C18—C19—C20	0.5 (3)	C62—C61—B3—C55	94.9 (3)
O5—C32—C31—N10	−6.7 (4)	C62—C61—B3—C49	−149.2 (3)
O5—C32—C31—C30	172.6 (3)	C62—C63—C64—C65	1.1 (5)
O5—C32—C33—C34	−1.4 (3)	C55—C60—C59—C58	0.3 (5)
O5—C35—C34—C33	0.0 (4)	C58—C57—C56—C55	1.3 (5)
O6—C39—C40—C41	−1.9 (4)	C9—C10—C11—O2	−144.8 (3)
O6—C42—C41—C40	−0.9 (4)	C9—C10—C11—C12	32.7 (4)
N3—N4—C10—C11	178.6 (2)	C57—C58—C59—C60	−1.4 (5)
N3—N4—C10—C9	0.7 (3)	C66—C61—C62—C63	−1.3 (4)
N3—C8—C9—C10	0.3 (3)	C66—C61—B3—C43	152.2 (3)
N8—N7—C22—C23	0.5 (3)	C66—C61—B3—C55	−83.5 (3)
N8—N7—B2—N11	−57.7 (3)	C66—C61—B3—C49	32.5 (4)
N8—N7—B2—N9	60.9 (3)	C66—C65—C64—C63	−1.4 (5)
N8—C24—C25—O4	3.0 (3)	C44—C43—B3—C61	−97.9 (3)
N8—C24—C25—C26	178.5 (3)	C44—C43—B3—C55	140.7 (3)
N8—C24—C23—C22	−1.0 (3)	C44—C43—B3—C49	24.9 (4)
N12—N11—C38—C37	−2.5 (3)	C44—C43—C48—C47	−2.9 (5)
N12—N11—C38—C39	174.0 (2)	C44—C45—C46—C47	−1.7 (5)
N12—N11—B2—N7	47.3 (3)	C23—C24—C25—O4	−171.0 (3)
N12—N11—B2—N9	−71.1 (3)	C23—C24—C25—C26	4.5 (6)

N12—C36—C37—C38	−0.7 (3)	C31—N10—N9—C29	−0.1 (3)
N7—N8—C24—C25	−174.0 (2)	C31—N10—N9—B2	176.8 (2)
N7—N8—C24—C23	1.3 (3)	C31—C32—C33—C34	176.2 (3)
N7—C22—C23—C24	0.3 (3)	C60—C55—C56—C57	−2.3 (4)
N4—N3—C8—C9	0.1 (3)	C60—C55—B3—C61	−133.9 (3)
N4—N3—B1—N1	−49.4 (3)	C60—C55—B3—C43	−12.0 (4)
N4—N3—B1—N5	71.2 (3)	C60—C55—B3—C49	105.2 (3)
N4—C10—C11—O2	37.6 (4)	C35—O5—C32—C31	−176.8 (2)
N4—C10—C11—C12	−144.9 (3)	C35—O5—C32—C33	1.4 (3)
N4—C10—C9—C8	−0.7 (3)	C29—N9—B2—N7	115.1 (3)
N6—N5—C15—C16	0.2 (3)	C29—N9—B2—N11	−126.1 (3)
N6—N5—B1—N3	−53.9 (3)	C45—C46—C47—C48	0.5 (5)
N6—N5—B1—N1	65.9 (3)	B1—N3—N4—Dy1	−18.2 (3)
N6—C17—C16—C15	0.2 (3)	B1—N3—N4—C10	−178.2 (2)
N6—C17—C18—O3	−2.9 (3)	B1—N3—C8—C9	177.7 (2)
N6—C17—C18—C19	176.0 (3)	B1—N1—C1—C2	179.0 (2)
N2—N1—C1—C2	0.8 (3)	B1—N5—C15—C16	−172.3 (3)
N2—N1—B1—N3	63.3 (3)	C54—C49—B3—C61	−157.7 (3)
N2—N1—B1—N5	−56.5 (3)	C54—C49—B3—C43	81.5 (3)
N2—C3—C2—C1	−0.8 (3)	C54—C49—B3—C55	−39.7 (3)
N11—N12—C36—C37	−0.7 (3)	C54—C49—C50—C51	2.0 (4)
N11—C38—C39—O6	150.8 (3)	C33—C32—C31—N10	175.8 (3)
N11—C38—C39—C40	−35.5 (5)	C33—C32—C31—C30	−5.0 (6)
N1—N2—C3—C4	−180.0 (2)	C64—C63—C62—C61	0.2 (5)
N1—N2—C3—C2	1.3 (3)	C42—O6—C39—C38	176.6 (3)
O2—C14—C13—C12	−0.8 (4)	C42—O6—C39—C40	1.4 (3)
N5—N6—C17—C16	−0.1 (3)	C56—C55—C60—C59	1.5 (4)
N5—N6—C17—C18	−179.7 (2)	C56—C55—B3—C61	51.4 (3)
N10—N9—C29—C30	−0.2 (3)	C56—C55—B3—C43	173.3 (3)
N10—N9—B2—N7	−61.1 (3)	C56—C55—B3—C49	−69.5 (3)
N10—N9—B2—N11	57.8 (3)	C59—C58—C57—C56	0.7 (5)
N10—C31—C30—C29	−0.5 (3)	C52—C51—C50—C49	−2.4 (5)
N9—N10—C31—C32	179.7 (2)	C49—C54—C53—C52	−2.0 (5)
N9—N10—C31—C30	0.3 (3)	C51—C52—C53—C54	1.7 (5)
N9—C29—C30—C31	0.4 (3)	B2—N7—C22—C23	−179.6 (3)
C36—N12—N11—C38	2.0 (3)	B2—N11—C38—C37	174.1 (3)
C36—N12—N11—B2	−175.0 (2)	B2—N11—C38—C39	−9.4 (4)
C36—C37—C38—N11	1.9 (3)	B2—N9—C29—C30	−176.7 (3)
C36—C37—C38—C39	−174.3 (3)	C53—C54—C49—B3	−174.9 (3)
C37—C38—C39—O6	−33.5 (4)	C53—C54—C49—C50	0.2 (4)
C37—C38—C39—C40	140.3 (4)	C53—C52—C51—C50	0.4 (5)
C4—O1—C7—C6	−0.8 (3)	B3—C61—C62—C63	−179.7 (3)
C4—C3—C2—C1	−179.6 (3)	B3—C61—C66—C65	179.5 (3)
C4—C5—C6—C7	−0.1 (3)	B3—C43—C44—C45	179.6 (3)
C3—N2—N1—C1	−1.3 (3)	B3—C43—C48—C47	179.3 (3)
C3—N2—N1—B1	−179.5 (2)	B3—C55—C60—C59	−173.5 (3)
C3—C4—C5—C6	179.7 (3)	B3—C55—C56—C57	172.9 (3)
C3—C2—C1—N1	0.0 (3)	B3—C49—C50—C51	176.8 (3)

C38—N11—B2—N7	−128.9 (3)	C50—C49—B3—C61	27.8 (4)
C38—N11—B2—N9	112.6 (3)	C50—C49—B3—C43	−93.0 (3)
C38—C39—C40—C41	−175.9 (3)	C50—C49—B3—C55	145.8 (3)
C21—O3—C18—C17	178.8 (2)	C48—C43—C44—C45	1.7 (4)
C21—O3—C18—C19	−0.4 (3)	C48—C43—B3—C61	79.7 (3)
C21—C20—C19—C18	−0.3 (3)	C48—C43—B3—C55	−41.7 (4)
C7—O1—C4—C3	−179.3 (2)	C48—C43—B3—C49	−157.4 (3)
C7—O1—C4—C5	0.8 (3)	C14—O2—C11—C10	179.1 (3)
C17—N6—N5—C15	−0.1 (3)	C14—O2—C11—C12	1.3 (3)
C17—N6—N5—B1	173.7 (2)	C13—C12—C11—O2	−1.8 (4)
C17—C16—C15—N5	−0.3 (3)	C13—C12—C11—C10	−179.5 (3)
C17—C18—C19—C20	−178.6 (3)		