

Bis[3-(anthracen-9-yl)pentane-2,4-dionato- κ^2O,O']- (N,N -dimethylformamide- κO)[tris(pyrazol-1-yl- κN^2)hydroborato]europium(III)

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Keywords: crystal structure; lanthanide complexes; luminescence; antenna ligands.

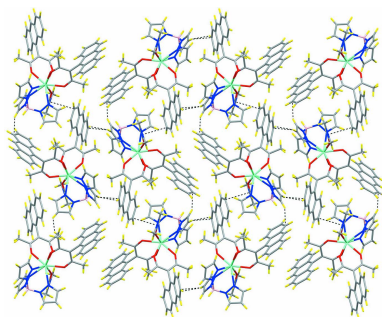
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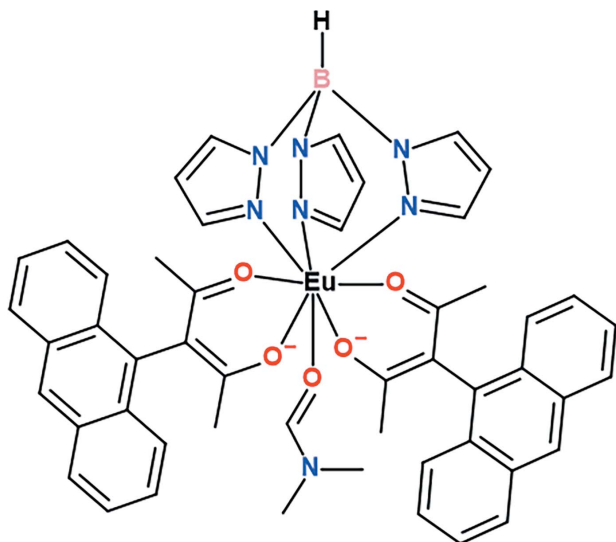
The title compound, [Eu(C₉H₁₀BN₆)(C₁₉H₁₅O₂)₂(C₃H₇NO)] or [TpEu(Anthracac)₂(DMF)], was synthesized by reaction of a tris(pyrazolyl)borate (Tp⁻) Eu³⁺ complex with 3-(anthracen-9-yl)pentane-2,4-dione (HAnthracac) in the presence of triethylamine. In the title compound, Eu³⁺ is located in an octavertex square-pyramidal coordination environment. In the two Anthracac⁻ ligands, the anthracene and nearly planar acetylacetonate fragments are almost orthogonal. Neighboring molecules of TpEu(Anthracac)₂(DMF) are connected in the crystal by intermolecular van der Waals interactions, while π -stacking interactions are limited to the edges of two anthracene rings.

1. Chemical context

Lanthanide complexes find numerous applications as, for example, luminescent materials, markers, security inks, components of lasers, light-emitting diodes, and many others (Bünzli, 2017; Venturini Filho *et al.*, 2018; Khullar *et al.*, 2019; Bünzli, 2019). This variety of uses relies in large parts on the electronic structure of the Ln³⁺ ions, which leads to electronic transitions occurring between *f*-orbitals, providing them with unique luminescence characteristics, including high color purity and exact reproducibility of the emitted light color (Sarkar *et al.*, 2019; Wang, Pu *et al.*, 2019; Wang, Zhao *et al.*, 2019). In spite of these advantages, the electronic structure of Ln³⁺ ions causes the luminescence to be of low intensity due to the forbidden nature of *f*-*f* electronic transitions (Bünzli, 2017; Zhang *et al.*, 2020; Wang, Zhao *et al.*, 2019), hence the weak absorbance of the exciting radiation. This feature is usually evaded by using organic ‘antenna’ ligands, which are capable of absorbing exciting radiation and transferring the gained energy to the Ln³⁺ ions (Bünzli, 2017; Carneiro Neto *et al.*, 2019; Aulsebrook *et al.*, 2018). Recently, it was shown (Mikhalyova *et al.*, 2017; Gheno *et al.*, 2014; Mikhalyova *et al.*, 2020; Bortoluzzi *et al.*, 2012) that tris(pyrazolyl)borate anions are efficient antenna ligands for Tb³⁺ and Eu³⁺, both exhibiting emission in the visible range. Anions of β -diketones with different substituents are also well-known antenna ligands (Wang, Zhao *et al.*, 2019; Nehra *et al.*, 2022). To increase the extinction coefficients of the ligands, it can be of advantage to add a large conjugated moiety to their structure. Recently it was found by us (Kandel *et al.*, 2017; Mikhalyova *et*



al., 2017), that the combination of several antenna ligands in one compound can have complex and unpredictable effects on its luminescence characteristics, which also depend on the molecular and crystal structure details of the complex. Thus, for this work, an Eu^{3+} complex with two types of antenna ligands, *i.e.* tris(pyrazolyl)borate (Tp^-) and 3-(anthracen-9-yl)pentane-2,4-dionate (Anthracac^-), of the composition $\text{TpEu}(\text{Anthracac})_2(\text{DMF})$ was obtained and its molecular and crystal structures were studied.



2. Structural commentary

The title compound is a neutral metal-containing complex and crystallizes in the monoclinic $P2_1/n$ space group with only one molecule in the asymmetric unit (Fig. 1). The unit cell contains two molecules of each enantiomer, whose crystallographic positions are related by the inversion centers, glide planes and screw axes (Fig. 2). The asymmetric unit consists of the Eu^{3+}

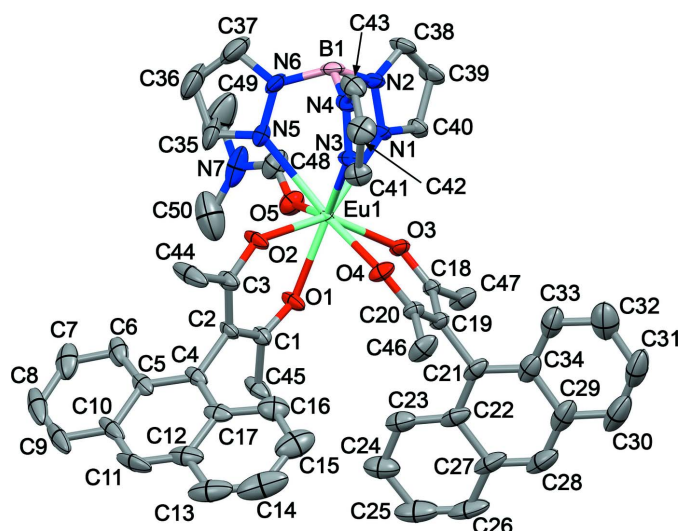


Figure 1
The molecular structure of the title compound. Atomic displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity of presentation.

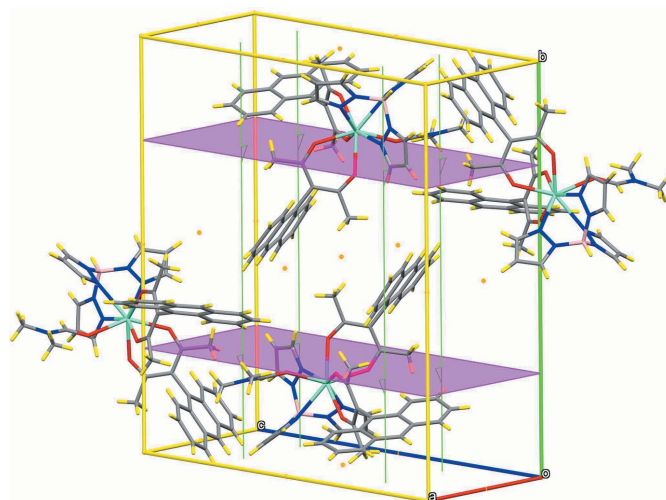


Figure 2
Stick diagram of a unit-cell view with symmetry elements: inversion centers (orange), glide planes (violet) and screw axes (green).

ion surrounded by one Tp^- and two Anthracac^- ligands and one dimethylformamide molecule. Of these ligands, the Tp^- is coordinated tridentately, donating three N atoms to the coordination polyhedron, while each Anthracac^- acts as a bidentate O ligand, donating a combined four O atoms. The DMF molecule acts as a unidentate O donor. As is typical for lanthanide ions with seven, eight or nine coordinating atoms, the assignment of the coordination geometry carries some ambiguity. Several different criteria have been proposed to define the shape of such a coordination polyhedron. Use of the *Shape 2.1* software (Casanova *et al.*, 2005; Alvarez *et al.*, 2005), indicates that the Eu^{3+} ion in the title compound is an octa-vertex with a slightly distorted square-antiprismatic geometry (Fig. 3), with a mean angle between the capping and basal square planes of the coordination polyhedron of $0.75 (8)^\circ$. According to the Lippard & Russ (1968) criterion, the angle between the body-diagonal trapezoids for the title compound, ω , is $88.24 (7)^\circ$, which is closer to the angle for a dodecahedron (90.0°) than a square antiprism (79.3°). A more accurate criterion is the one proposed by Porai-Koshits and Aslanov

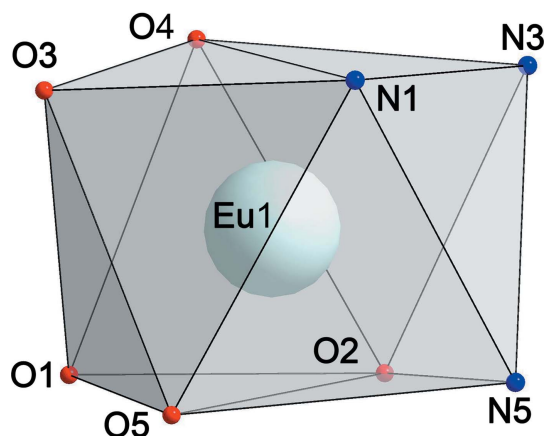


Figure 3
The geometry of the Eu^{3+} coordination polyhedron.

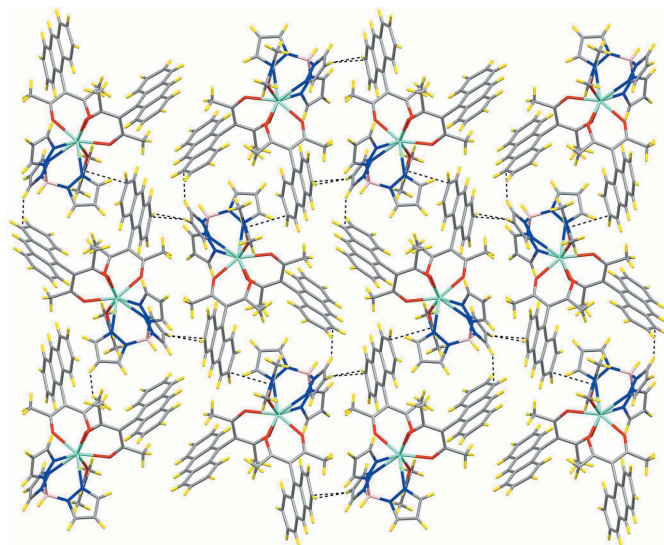


Figure 4
Packing view along the *a*-axis (see also Fig. S3).

(1972) based on the angles, δ , between pairs of faces intersecting along the edges connecting the vertices where the five edges intersect. The respective angles for the complex here are 6.6 (1), 8.9 (1), 43.3 (1), and 49.7 (1) $^\circ$ and the degrees of non-planarity of the diagonal trapezoids, φ , are 18.81 (9) and 19.74 (1) $^\circ$. From these criteria, the δ angles are closer to those of an idealized square antiprism, yet the φ angles correspond to those of a bicapped trigonal prism. Thus, three different criteria define three different polyhedra and among these criteria, only the δ -based one agrees with the assignment using the *Shape 2.1* software.

The lengths for Eu-donor atom bonds are listed in Table 1 and these are in the usual range for compounds with similar ligands (Mikhalyova *et al.*, 2020; Lawrence *et al.*, 2001; Dei *et al.*, 2000).

Regarding the geometrical features of the ligands, it should be noted that the planar anthracene moiety and the nearly planar acetylacetonate fragment are almost orthogonal to

Table 1
Selected bond lengths (\AA).

Eu1—O1	2.351 (3)	Eu1—O5	2.417 (3)
Eu1—O2	2.313 (3)	Eu1—N1	2.582 (3)
Eu1—O3	2.344 (3)	Eu1—N3	2.555 (3)
Eu1—O4	2.340 (3)	Eu1—N5	2.573 (3)

Table 2
Selected intermolecular interatomic distances (\AA).

C8...C15 ⁱ	3.258 (8)	C8...H36 ⁱⁱ	2.698
H8...C15 ⁱ	2.817	H37...C26 ⁱⁱⁱ	2.830
H50C...N3 ⁱ	2.680	C48...C14 ⁱⁱⁱ	3.159 (8)
H50C...C41 ⁱ	2.718		

Symmetry codes: (i) $-1 + x, y, z$; (ii) $x, 2 - y, 1 - z$; (iii) $-\frac{1}{2} + x, \frac{3}{2} - y, -\frac{1}{2} + z$.

each other in each Anthracac⁻ ligand, subtending dihedral angles of 87.84 (7) and 79.98 (7) $^\circ$. This is due to the presence of the CH₃ groups, which prevent rotation of the anthracenyl fragments along the C2—C4 and C19—C21 bonds.

3. Supramolecular features

The crystal packing of the title compound consists of separate neutral molecules. Several short contacts are observed (Table 2), but none of these exhibit the typical characteristics of directional attractive interactions, *i.e.* they are not hydrogen bonds or C—H... π interactions. It thus can be said that these molecules are organized in the lattice predominantly by intermolecular van der Waals or dispersion interactions (Fig. 4, Table 2).

π -Stacking interactions play no dominant role in this structure. For one of the anthracene fragments (C4—C16) no π - π stacking interactions are observed at all. For the other anthracenyl group (C21—C34) one π -interaction is present, but it is limited to part of one of the outer phenylene groups, C29—C34, which is π -stacked with its inversion-related counterpart [symmetry code: (i) $2 - x, 1 - y, 1 - z$], with a centroid-to-centroid distance of 3.958 (8) \AA (Fig. 5). The remainder of the

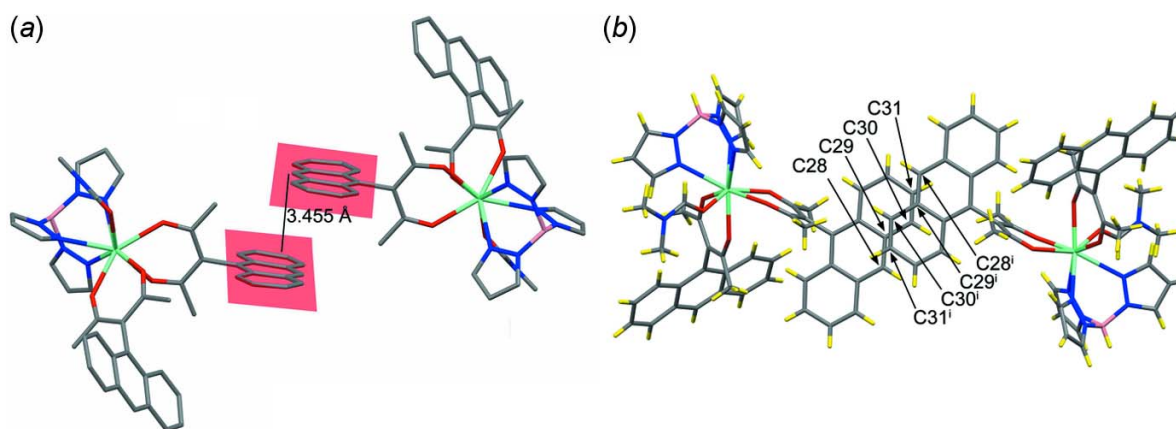


Figure 5
(a) View of the π - π stacking interaction observed for one of the phenylene groups of the anthracene fragments and (b) a view of the same, perpendicular to the planes of the anthracenyl (C21—C34) fragments [symmetry code: (i) $2 - x, 1 - y, 1 - z$]. Other occurrences of parallel (but not stacked) anthracenyl units are shown in Figs. S1, S2 and S4.

Table 3
Experimental details.

Crystal data	
Chemical formula	[Eu(C ₉ H ₁₀ BN ₆)(C ₁₉ H ₁₅ O ₂) ₂ (C ₃ H ₇ NO)]
<i>M_r</i>	988.71
Crystal system, space group	Monoclinic, <i>P2₁/n</i>
Temperature (K)	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.3728 (3), 22.5555 (7), 22.0840 (6)
β (°)	96.314 (3)
<i>V</i> (Å ³)	4640.4 (2)
<i>Z</i>	4
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	10.11
Crystal size (mm)	0.48 × 0.18 × 0.12
Data collection	
Diffraction	Rigaku Oxford Diffraction Gemini Eos
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.163, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	19671, 8850, 7261
<i>R_{int}</i>	0.048
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.615
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.042, 0.106, 1.03
No. of reflections	8850
No. of parameters	583
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	1.09, -1.25

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2020), and *pubCIF* (Westrip, 2010).

anthracenyl group does not participate in the π - π stacking interaction; for the entire anthracene moiety (C21–C34) the distance between the centroids is 6.006 (8) Å. The distance between inversion-related mean planes (C21–C34 and C21ⁱ–C34ⁱ) is 3.455 Å, indicating a medium strength stacking interaction (Fig. 5).

4. Database survey

The Cambridge Structural Database (CSD, version 5.41, updates till Aug 2020; Groom *et al.*, 2016) contains just one crystal structure with an Ln³⁺ ion surrounded by two β -diketonate anions and one tris(pyrazolyl)borate ligand, namely, bis(1,3-diphenyl-1,3-propanedionato-*O,O'*){hydrotris[3-(2-pyridyl)-pyrazol-1-yl]borato}praseodymium(III) (FOLZUC; Davies *et al.*, 2005). However, in this compound the Pr³⁺ ion is deca-coordinate owing to the presence of 2-pyridyl substituents in the tris(pyrazolyl)borate ligand, so a direct comparison of the coordination geometries of this and the title compound is not possible.

Fragments containing one Ln ion surrounded by at least one β -diketonate anion and one tris(pyrazolyl)borate ligand encompass 34 entities (including FOLZUC). Most of them (28), contain eight-coordinate lanthanide ions with two tris(pyrazolyl)borate ligands and one β -diketonate anion: DULWEP, DULWIT, DULWOZ, DULWUF, DULXAM,

DULXEQ, DULXIU, DULXOA, DULXUG, DULYAN, DULYER, DULYIV, DULYOB, DULYUH, DULZAO, DULZES, DULZIW, DULZOC, DULZUI and DUMDAT (all Mikhalyova *et al.*, 2020); ESUHOP (Galler *et al.*, 2004); GIFCUT, GIFDAA (Moss *et al.*, 1988); GIFCUT10, GIFDAA10 (Moss *et al.*, 1989); KIFKUI (Guégan *et al.*, 2018); XICHIA (Lawrence *et al.*, 2001). Again, the coordination environment of these compounds and the title one cannot be directly compared. One of the compounds, FOLZUC, is discussed above and another, [tris(3-*t*-butyl-5-methylpyrazolyl)hydroborato](2,2,6,6-tetramethylheptane-3,5-dionato)-ytterbium(II) (ESUJIL; Morissette *et al.*, 2004) is a neutral molecule of Yb²⁺. Four entities are complexes with salicylaldehyde derivatives [JAJRAO (Onishi *et al.*, 2004), QIDGAL, QIDGAL01 (Onishi *et al.*, 1999), and ZUCCI (Lawrence *et al.*, 1996)], which are also β -diketonate anions, but, again, compounds with these anions contain eight-coordinate Ln³⁺ ions.

Only three metal-containing structures were found with 3-naphthyl or 3-anthracenyl substituents. The interplanar angles for acetylacetonate *vs* aryl fragments are 86.4° for [3-(1'-naphthyl)pentane-2,4-dionato][tris(2-aminoethyl)amine]cobalt(III) bis(tetrafluoroborate) dihydrate, 87.1° for [3-(2',4'-dinitro-1'-naphthyl)pentane-2,4-dionato][tris(2-aminoethyl)amine]cobalt(III) dibromide (BEYTEE and BIMLUE, respectively; Nakano & Sato, 1982) and 83.5° for [3-(9'-anthryl)acetylacetonato]chlorido(1,4,7-trimethyl-1,4,7-triazacyclononane)iron(III) perchlorate mesitylene solvate (NUCZUG; Müller *et al.*, 1998). These angles are in the same range as for the title compound.

5. Synthesis and crystallization

The starting Tp₂EuCl complex was obtained by reaction of TpTl with EuCl₃·6H₂O in methanol (Kandel *et al.*, 2017). Then, 307 mg (0.50 mmol) of Tp₂EuCl and 138 mg (0.50 mmol) of HAnthracac were dissolved in 15 mL of methylene chloride, followed by the addition of 0.15 mL of triethylamine. After the solution had been stirred for 1 h, the reaction mixture was filtered and the filtrate was evaporated under reduced pressure (rotavapor). The resulting residue was washed with water and dried in a vacuum desiccator over P₂O₅. The crude product was recrystallized by slow diffusion of methyl *t*-butyl ether into a DMF solution of the compound. The title compound was obtained as orange prismatic crystals (25 mg, yield 10%).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. C–H bond distances were constrained to 0.95 Å for aromatic and alkene C–H moieties, and to 0.98 Å for CH₃ moieties. The B–H bond distance was constrained to 1.00 Å. *U*_{iso}(H) values were set to *kU*_{eq}(C) where *k* = 1.5 for CH₃ and 1.2 for C–H units.

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References

- Alvarez, S., Alemany, P., Casanova, D., Cirera, J., Lluell, M. & Avnir, D. (2005). *Coord. Chem. Rev.* **249**, 1693–1708.
- Aulsebrook, M. L., Graham, B., Grace, M. R. & Tuck, K. L. (2018). *Coord. Chem. Rev.* **375**, 191–220.
- Bortoluzzi, M., Paolucci, G., Gatto, M., Roppa, S., Enrichi, F., Ciorba, S. & Richards, B. S. (2012). *J. Lumin.* **132**, 2378–2384.
- Bünzli, J.-C. G. (2017). *Eur. J. Inorg. Chem.* pp. 5058–5063.
- Bünzli, J.-C. G. (2019). *Trends Chem.* **1**, 751–762.
- Carneiro Neto, A. N., Teotonio, E. E. S., de Sá, G. F., Brito, H. F., Legendziewicz, J., Carlos, L. D., Felinto, M. C. F. C., Gawryszewska, P., Moura, R. T. Jr, Longo, R. L., Faustino, W. M. & Malta, O. L. (2019). *Handbook on the Physics and Chemistry of Rare Earths*, vol. 56, pp. 55–162. Amsterdam: Elsevier.
- Casanova, D., Lluell, M., Alemany, P. & Alvarez, S. (2005). *Chem. Eur. J.* **11**, 1479–1494.
- Davies, G. M., Adams, H. & Ward, M. D. (2005). *Acta Cryst.* **C61**, m221–m223.
- Dei, A., Gatteschi, D., Massa, C. A., Pardi, L. A., Poussereau, S. & Sorace, L. (2000). *Chem. Eur. J.* **6**, 4580–4586.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Galler, J. L., Goodchild, S., Gould, J., McDonald, R. & Sella, A. (2004). *Polyhedron*, **23**, 253–262.
- Gheno, G., Bortoluzzi, M., Ganzerla, R. & Enrichi, F. (2014). *J. Lumin.* **145**, 963–969.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Guégan, F., Riobé, F., Maury, O., Jung, J., Le Guennic, B., Morell, C. & Luneau, D. (2018). *Inorg. Chem. Front.* **5**, 1346–1353.
- Kandel, A. V., Mikhalyova, E. A., Zeller, M., Addison, A. W. & Pavlishchuk, V. V. (2017). *Theor. Exp. Chem.* **53**, 180–186.
- Khullar, S., Singh, S., Das, P. & Mandal, S. K. (2019). *ACS Omega*, **4**, 5283–5292.
- Lawrence, R. G., Hamor, T. A., Jones, C. J., Paxton, K. & Rowley, N. M. (2001). *J. Chem. Soc. Dalton Trans.* pp. 2121–2126.
- Lawrence, R. G., Jones, C. J. & Kresinski, R. A. (1996). *J. Chem. Soc. Dalton Trans.* pp. 501–507.
- Lippard, S. L. & Russ, B. I. (1968). *Inorg. Chem.* **7**, 1686–1688.
- Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
- Mikhalyova, E. A., Yakovenko, A. V., Zeller, M., Gavrilenko, K. S., Kiskin, M. A., Smola, S. S., Dotsenko, V. P., Eremenko, I. L., Addison, A. W. & Pavlishchuk, V. V. (2017). *Dalton Trans.* **46**, 3457–3469.
- Mikhalyova, E. A., Zeller, M., Jasinski, J. P., Butcher, R. J., Carrella, L. M., Sedykh, A. E., Gavrilenko, K. S., Smola, S. S., Frasso, M., Cazorla, S. C., Perera, K., Shi, A., Ranjbar, H. G., Smith, C., Deac, A., Liu, Y., McGee, S. M., Dotsenko, V. P., Kumke, M. U., Müller-Buschbaum, K., Rentschler, E., Addison, A. W. & Pavlishchuk, V. V. (2020). *Dalton Trans.* **49**, 7774–7789.
- Morissette, M., Haufe, S., McDonald, R., Ferrence, G. M. & Takats, J. (2004). *Polyhedron*, **23**, 263–271.
- Moss, M. A. J., Jones, C. J. & Edwards, A. J. (1988). *Polyhedron*, **7**, 79–81.
- Moss, M. A. J., Jones, C. J. & Edwards, A. J. (1989). *J. Chem. Soc. Dalton Trans.* pp. 1393–1400.
- Müller, M., Weyhermüller, T., Bill, E. & Wieghardt, K. (1998). *J. Biol. Inorg. Chem.* **3**, 96–106.
- Nakano, Y. & Sato, S. (1982). *Inorg. Chem.* **21**, 1315–1318.
- Nehra, K., Dalal, A., Hooda, A., Bhagwan, S., Saini, R. K., Mari, B., Kumar, S. & Singh, D. (2022). *J. Mol. Struct.* **1249**, 131531.
- Onishi, M., Kayano, K., Inada, K., Yamaguchi, H., Nagaoka, J., Arikawa, Y. & Takatani, T. (2004). *Inorg. Chim. Acta*, **357**, 4091–4101.
- Onishi, M., Yamaguchi, H., Shimotsuma, H., Hiraki, K., Nagaoka, J. & Kawano, H. (1999). *Chem. Lett.* **28**, 573–574.
- Porai-Koshits, M. A. & Aslanov, L. A. (1972). *J. Struct. Chem.* **13**, 244–253.
- Rigaku OD (2015). *CrysAlisPro*. Rigaku Oxford Diffraction, Yarnton, England.
- Sarkar, D., Ganguli, S., Samanta, T. & Mahalingam, V. (2019). *Langmuir*, **35**, 6211–6230.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Venturini Filho, E., de Sousa Filho, P. C., Serra, O. A., Weber, I. T., Lucena, M. A. M. & Luz, P. P. (2018). *J. Lumin.* **202**, 89–96.
- Wang, F., Pu, Y., Zhang, X., Zhang, F., Cheng, H. & Zhao, Y. (2019). *J. Lumin.* **206**, 192–198.
- Wang, L., Zhao, Z., Wei, C., Wei, H., Liu, Z., Bian, Z. & Huang, C. (2019). *Adv. Opt. Mater.* **7**, 1801256.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Zhang, H., Chen, Z.-H., Liu, X. & Zhang, F. (2020). *Nano Res.* **13**, 1795–1809.

supporting information

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: ShelXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009), and *publCIF* (Westrip, 2010).

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Crystal data

[Eu(C₉H₁₀BN₆)(C₁₉H₁₅O₂)₂(C₃H₇NO)]
M_r = 988.71
 Monoclinic, *P2₁/n*
a = 9.3728 (3) Å
b = 22.5555 (7) Å
c = 22.0840 (6) Å
 β = 96.314 (3)°
V = 4640.4 (2) Å³
Z = 4

F(000) = 2016
D_x = 1.415 Mg m⁻³
 Cu *K* α radiation, λ = 1.54184 Å
 Cell parameters from 8094 reflections
 θ = 4.0–71.4°
 μ = 10.11 mm⁻¹
T = 173 K
 Prism, orange
 0.48 × 0.18 × 0.12 mm

Data collection

Rigaku Oxford Diffraction Gemini Eos
 diffractometer
 Radiation source: fine-focus sealed X-ray tube,
 Enhance (Cu) X-ray Source
 Graphite monochromator
 Detector resolution: 16.0416 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan
 (CrysAlisPro; Rigaku OD, 2015)

T_{min} = 0.163, *T_{max}* = 1.000
 19671 measured reflections
 8850 independent reflections
 7261 reflections with *I* > 2 σ (*I*)
R_{int} = 0.048
 θ_{max} = 71.4°, θ_{min} = 3.9°
h = -11→11
k = -27→17
l = -26→24

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2 σ (*F*²)] = 0.042
wR(*F*²) = 0.106

S = 1.03
 8850 reflections
 583 parameters
 0 restraints

Primary atom site location: dual
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 1.09 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.25 \text{ e } \text{\AA}^{-3}$

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Eu1	0.52702 (2)	0.81156 (2)	0.43393 (2)	0.01770 (8)
O1	0.4093 (3)	0.77371 (12)	0.51430 (12)	0.0316 (6)
O2	0.4941 (4)	0.88721 (12)	0.50175 (13)	0.0396 (8)
O3	0.5692 (3)	0.70993 (11)	0.42273 (11)	0.0263 (6)
O4	0.7264 (3)	0.78408 (11)	0.50130 (13)	0.0317 (6)
O5	0.2953 (3)	0.77901 (14)	0.38675 (14)	0.0383 (7)
N1	0.5855 (4)	0.79579 (14)	0.32351 (13)	0.0248 (7)
N2	0.6057 (4)	0.83970 (15)	0.28333 (14)	0.0294 (7)
N3	0.7242 (4)	0.88341 (14)	0.41029 (14)	0.0266 (7)
N4	0.7259 (4)	0.91415 (14)	0.35743 (14)	0.0268 (7)
N5	0.4131 (4)	0.89911 (15)	0.37142 (16)	0.0331 (8)
N6	0.4623 (4)	0.92238 (15)	0.32156 (16)	0.0361 (8)
N7	0.0779 (5)	0.7911 (2)	0.3344 (3)	0.0597 (14)
C1	0.3798 (4)	0.79077 (17)	0.56538 (18)	0.0266 (8)
C2	0.4045 (5)	0.84859 (17)	0.58988 (17)	0.0269 (8)
C3	0.4583 (5)	0.89398 (18)	0.55457 (19)	0.0339 (10)
C4	0.3751 (5)	0.86189 (16)	0.65368 (18)	0.0298 (9)
C5	0.2383 (5)	0.88156 (16)	0.6657 (2)	0.0345 (10)
C6	0.1212 (5)	0.88699 (18)	0.6203 (2)	0.0424 (11)
H6	0.1357	0.8791	0.5792	0.051*
C7	-0.0128 (6)	0.9033 (2)	0.6333 (3)	0.0591 (16)
H7	-0.0900	0.9063	0.6018	0.071*
C8	-0.0347 (9)	0.9156 (2)	0.6950 (4)	0.079 (3)
H8	-0.1274	0.9266	0.7046	0.094*
C9	0.0737 (9)	0.9117 (2)	0.7394 (3)	0.071 (2)
H9	0.0562	0.9201	0.7800	0.085*
C10	0.2147 (7)	0.89522 (18)	0.7277 (2)	0.0496 (15)
C11	0.3259 (8)	0.8903 (2)	0.7737 (2)	0.0584 (18)
H11	0.3095	0.9007	0.8140	0.070*
C12	0.4595 (7)	0.87091 (19)	0.7630 (2)	0.0501 (14)
C13	0.5756 (10)	0.8643 (2)	0.8103 (3)	0.072 (2)
H13	0.5615	0.8757	0.8506	0.086*
C14	0.7041 (10)	0.8424 (3)	0.7996 (3)	0.084 (3)
H14	0.7790	0.8385	0.8320	0.101*

C15	0.7271 (7)	0.8252 (3)	0.7400 (3)	0.0683 (19)
H15	0.8169	0.8088	0.7328	0.082*
C16	0.6219 (6)	0.8320 (2)	0.6926 (2)	0.0471 (12)
H16	0.6406	0.8211	0.6527	0.056*
C17	0.4842 (5)	0.85520 (18)	0.70201 (19)	0.0360 (10)
C18	0.6316 (5)	0.66956 (16)	0.45555 (16)	0.0250 (8)
C19	0.7273 (4)	0.67949 (16)	0.50837 (16)	0.0253 (8)
C20	0.7690 (4)	0.73674 (18)	0.52778 (17)	0.0271 (8)
C21	0.7840 (5)	0.62631 (17)	0.54511 (18)	0.0353 (10)
C22	0.6957 (6)	0.59931 (18)	0.58541 (19)	0.0417 (12)
C23	0.5594 (6)	0.6217 (2)	0.5950 (2)	0.0448 (12)
H23	0.5257	0.6567	0.5741	0.054*
C24	0.4744 (7)	0.5949 (3)	0.6332 (2)	0.0580 (15)
H24	0.3843	0.6118	0.6394	0.070*
C25	0.5201 (10)	0.5420 (3)	0.6635 (3)	0.075 (2)
H25	0.4595	0.5229	0.6892	0.090*
C26	0.6484 (9)	0.5188 (2)	0.6562 (2)	0.0654 (19)
H26	0.6768	0.4828	0.6765	0.079*
C27	0.7442 (7)	0.5466 (2)	0.6185 (2)	0.0503 (14)
C28	0.8772 (7)	0.5250 (2)	0.6124 (2)	0.0587 (17)
H28	0.9088	0.4905	0.6347	0.070*
C29	0.9690 (7)	0.5512 (2)	0.5747 (2)	0.0540 (15)
C30	1.1070 (8)	0.5289 (3)	0.5678 (3)	0.074 (2)
H30	1.1411	0.4948	0.5903	0.089*
C31	1.1914 (8)	0.5550 (3)	0.5299 (3)	0.071 (2)
H31	1.2842	0.5391	0.5269	0.085*
C32	1.1462 (7)	0.6054 (3)	0.4942 (3)	0.0692 (19)
H32	1.2067	0.6229	0.4674	0.083*
C33	1.0122 (6)	0.6281 (2)	0.4999 (2)	0.0511 (13)
H33	0.9806	0.6620	0.4764	0.061*
C34	0.9201 (6)	0.6030 (2)	0.5391 (2)	0.0434 (12)
C35	0.2815 (6)	0.9201 (2)	0.3731 (3)	0.0520 (13)
H35	0.2225	0.9118	0.4043	0.062*
C36	0.2421 (8)	0.9556 (3)	0.3235 (4)	0.076 (2)
H36	0.1529	0.9753	0.3135	0.091*
C37	0.3605 (7)	0.9565 (3)	0.2915 (3)	0.0662 (17)
H37	0.3686	0.9774	0.2547	0.079*
C38	0.6116 (6)	0.8170 (2)	0.22766 (18)	0.0374 (10)
H38	0.6252	0.8389	0.1920	0.045*
C39	0.5948 (5)	0.7566 (2)	0.23078 (18)	0.0373 (10)
H39	0.5933	0.7287	0.1985	0.045*
C40	0.5805 (5)	0.74553 (18)	0.29162 (17)	0.0282 (8)
H40	0.5688	0.7072	0.3083	0.034*
C41	0.8332 (5)	0.9041 (2)	0.4480 (2)	0.0384 (10)
H41	0.8576	0.8906	0.4886	0.046*
C42	0.9064 (6)	0.9479 (2)	0.4203 (2)	0.0476 (12)
H42	0.9882	0.9695	0.4372	0.057*
C43	0.8344 (6)	0.95314 (19)	0.3629 (2)	0.0410 (11)

H43	0.8576	0.9799	0.3323	0.049*
C44	0.4746 (8)	0.9563 (2)	0.5808 (2)	0.067 (2)
H44A	0.5506	0.9772	0.5623	0.101*
H44B	0.4998	0.9540	0.6250	0.101*
H44C	0.3839	0.9778	0.5720	0.101*
C45	0.3115 (6)	0.74539 (18)	0.6032 (2)	0.0405 (11)
H45A	0.2855	0.7102	0.5783	0.061*
H45B	0.2251	0.7623	0.6177	0.061*
H45C	0.3796	0.7342	0.6382	0.061*
C46	0.8711 (6)	0.7442 (2)	0.5854 (2)	0.0445 (12)
H46A	0.9668	0.7302	0.5782	0.067*
H46B	0.8363	0.7211	0.6183	0.067*
H46C	0.8762	0.7862	0.5968	0.067*
C47	0.5960 (6)	0.60688 (18)	0.43470 (19)	0.0394 (11)
H47A	0.5374	0.5879	0.4633	0.059*
H47B	0.6850	0.5844	0.4333	0.059*
H47C	0.5424	0.6078	0.3940	0.059*
C48	0.2187 (6)	0.7920 (2)	0.3402 (3)	0.0481 (12)
H48	0.2645	0.8035	0.3057	0.058*
C49	-0.0009 (10)	0.8083 (3)	0.2768 (4)	0.106 (4)
H49A	0.0668	0.8210	0.2485	0.158*
H49B	-0.0658	0.8412	0.2835	0.158*
H49C	-0.0568	0.7745	0.2594	0.158*
C50	-0.0025 (8)	0.7747 (4)	0.3832 (4)	0.094 (3)
H50A	0.0636	0.7644	0.4192	0.141*
H50B	-0.0630	0.7404	0.3709	0.141*
H50C	-0.0632	0.8079	0.3929	0.141*
B1	0.6109 (6)	0.9057 (2)	0.3029 (2)	0.0331 (11)
H1	0.6336	0.9311	0.2681	0.040*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Eu1	0.02659 (12)	0.01614 (10)	0.01118 (10)	0.00364 (9)	0.00566 (7)	-0.00032 (7)
O1	0.0516 (18)	0.0232 (13)	0.0240 (13)	-0.0069 (12)	0.0212 (13)	-0.0064 (10)
O2	0.079 (2)	0.0166 (12)	0.0292 (14)	-0.0018 (14)	0.0342 (15)	-0.0044 (10)
O3	0.0391 (15)	0.0230 (12)	0.0160 (11)	0.0072 (11)	-0.0003 (11)	0.0018 (10)
O4	0.0422 (17)	0.0186 (12)	0.0318 (14)	-0.0022 (12)	-0.0072 (13)	0.0049 (11)
O5	0.0329 (16)	0.0390 (16)	0.0406 (17)	-0.0004 (13)	-0.0067 (14)	0.0018 (13)
N1	0.0393 (19)	0.0235 (15)	0.0127 (13)	0.0060 (13)	0.0075 (13)	-0.0013 (11)
N2	0.046 (2)	0.0281 (17)	0.0149 (14)	0.0025 (15)	0.0055 (14)	0.0022 (12)
N3	0.0397 (19)	0.0229 (14)	0.0178 (14)	-0.0003 (14)	0.0060 (14)	0.0029 (12)
N4	0.0397 (19)	0.0201 (14)	0.0225 (15)	-0.0010 (14)	0.0123 (14)	-0.0017 (12)
N5	0.037 (2)	0.0259 (16)	0.0366 (19)	0.0130 (15)	0.0052 (16)	0.0034 (14)
N6	0.050 (2)	0.0284 (17)	0.0277 (17)	0.0182 (16)	-0.0042 (16)	0.0058 (13)
N7	0.039 (2)	0.041 (2)	0.094 (4)	0.0157 (19)	-0.021 (3)	-0.021 (2)
C1	0.033 (2)	0.0217 (17)	0.0267 (18)	-0.0019 (15)	0.0119 (16)	-0.0023 (15)
C2	0.040 (2)	0.0227 (17)	0.0206 (17)	0.0004 (16)	0.0159 (16)	-0.0031 (14)

C3	0.056 (3)	0.0205 (18)	0.028 (2)	-0.0003 (18)	0.019 (2)	-0.0025 (15)
C4	0.048 (2)	0.0183 (17)	0.0268 (19)	-0.0071 (17)	0.0188 (18)	-0.0059 (14)
C5	0.054 (3)	0.0143 (16)	0.040 (2)	-0.0052 (17)	0.028 (2)	-0.0038 (15)
C6	0.047 (3)	0.0206 (18)	0.064 (3)	-0.0014 (19)	0.027 (2)	-0.0067 (19)
C7	0.050 (3)	0.024 (2)	0.108 (5)	0.000 (2)	0.028 (3)	-0.001 (3)
C8	0.092 (5)	0.022 (2)	0.140 (7)	0.009 (3)	0.090 (5)	0.010 (3)
C9	0.115 (6)	0.019 (2)	0.093 (5)	0.007 (3)	0.085 (5)	0.000 (3)
C10	0.091 (4)	0.0167 (18)	0.051 (3)	-0.005 (2)	0.052 (3)	-0.0055 (17)
C11	0.127 (6)	0.028 (2)	0.027 (2)	-0.016 (3)	0.040 (3)	-0.0104 (17)
C12	0.101 (5)	0.023 (2)	0.028 (2)	-0.017 (2)	0.013 (3)	-0.0027 (16)
C13	0.146 (7)	0.031 (3)	0.034 (3)	-0.028 (4)	-0.007 (4)	0.002 (2)
C14	0.126 (7)	0.053 (4)	0.062 (4)	-0.045 (4)	-0.045 (5)	0.017 (3)
C15	0.063 (4)	0.057 (3)	0.079 (4)	-0.022 (3)	-0.015 (3)	0.023 (3)
C16	0.049 (3)	0.045 (3)	0.047 (3)	-0.016 (2)	0.006 (2)	0.005 (2)
C17	0.059 (3)	0.0224 (18)	0.028 (2)	-0.0147 (19)	0.011 (2)	0.0014 (15)
C18	0.039 (2)	0.0197 (17)	0.0168 (16)	0.0072 (16)	0.0052 (15)	-0.0013 (13)
C19	0.035 (2)	0.0214 (17)	0.0191 (16)	0.0052 (15)	0.0000 (15)	0.0017 (13)
C20	0.029 (2)	0.0293 (19)	0.0221 (17)	0.0038 (16)	-0.0012 (16)	0.0035 (15)
C21	0.054 (3)	0.0222 (18)	0.0261 (19)	0.0072 (18)	-0.0128 (19)	-0.0028 (15)
C22	0.075 (4)	0.0229 (19)	0.0226 (19)	-0.002 (2)	-0.012 (2)	0.0012 (15)
C23	0.066 (3)	0.035 (2)	0.033 (2)	-0.005 (2)	-0.001 (2)	0.0079 (18)
C24	0.080 (4)	0.052 (3)	0.042 (3)	-0.017 (3)	0.009 (3)	0.010 (2)
C25	0.114 (6)	0.059 (4)	0.050 (3)	-0.029 (4)	0.001 (4)	0.022 (3)
C26	0.115 (6)	0.034 (3)	0.043 (3)	-0.016 (3)	-0.012 (3)	0.019 (2)
C27	0.087 (4)	0.025 (2)	0.034 (2)	0.004 (2)	-0.018 (3)	0.0059 (18)
C28	0.102 (5)	0.029 (2)	0.040 (3)	0.015 (3)	-0.017 (3)	0.003 (2)
C29	0.070 (4)	0.041 (3)	0.044 (3)	0.024 (3)	-0.026 (3)	-0.017 (2)
C30	0.090 (5)	0.055 (3)	0.068 (4)	0.038 (4)	-0.033 (4)	-0.012 (3)
C31	0.066 (4)	0.071 (4)	0.069 (4)	0.040 (4)	-0.023 (3)	-0.019 (3)
C32	0.057 (4)	0.089 (5)	0.058 (4)	0.017 (3)	-0.010 (3)	-0.028 (3)
C33	0.051 (3)	0.048 (3)	0.050 (3)	0.020 (2)	-0.011 (2)	-0.013 (2)
C34	0.056 (3)	0.034 (2)	0.036 (2)	0.014 (2)	-0.014 (2)	-0.0124 (18)
C35	0.044 (3)	0.032 (2)	0.080 (4)	0.022 (2)	0.007 (3)	0.005 (2)
C36	0.061 (4)	0.056 (4)	0.109 (6)	0.033 (3)	0.000 (4)	0.020 (4)
C37	0.076 (4)	0.051 (3)	0.068 (4)	0.023 (3)	-0.007 (3)	0.024 (3)
C38	0.056 (3)	0.042 (2)	0.0161 (17)	-0.004 (2)	0.0130 (18)	0.0007 (16)
C39	0.056 (3)	0.039 (2)	0.0193 (18)	-0.003 (2)	0.0113 (19)	-0.0079 (16)
C40	0.037 (2)	0.0282 (19)	0.0200 (18)	0.0001 (17)	0.0070 (16)	-0.0047 (14)
C41	0.044 (3)	0.036 (2)	0.034 (2)	-0.006 (2)	-0.002 (2)	-0.0020 (17)
C42	0.051 (3)	0.036 (2)	0.056 (3)	-0.014 (2)	0.005 (2)	-0.004 (2)
C43	0.057 (3)	0.027 (2)	0.042 (2)	-0.009 (2)	0.021 (2)	-0.0025 (17)
C44	0.140 (6)	0.023 (2)	0.049 (3)	-0.020 (3)	0.060 (4)	-0.012 (2)
C45	0.062 (3)	0.0257 (19)	0.040 (2)	-0.014 (2)	0.032 (2)	-0.0065 (17)
C46	0.054 (3)	0.031 (2)	0.042 (3)	0.002 (2)	-0.023 (2)	-0.0043 (18)
C47	0.064 (3)	0.0226 (19)	0.028 (2)	0.003 (2)	-0.011 (2)	-0.0035 (15)
C48	0.051 (3)	0.035 (2)	0.056 (3)	0.006 (2)	-0.007 (2)	-0.004 (2)
C49	0.100 (6)	0.077 (5)	0.125 (7)	0.032 (5)	-0.056 (6)	-0.029 (5)
C50	0.062 (4)	0.090 (6)	0.135 (8)	-0.007 (4)	0.035 (5)	-0.044 (5)

B1	0.057 (3)	0.026 (2)	0.0174 (19)	0.004 (2)	0.008 (2)	0.0094 (16)
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Geometric parameters (Å, °)

Eu1—O1	2.351 (3)	C20—C46	1.515 (5)
Eu1—O2	2.313 (3)	C21—C22	1.418 (7)
Eu1—O3	2.344 (3)	C21—C34	1.399 (7)
Eu1—O4	2.340 (3)	C22—C23	1.411 (8)
Eu1—O5	2.417 (3)	C22—C27	1.443 (6)
Eu1—N1	2.582 (3)	C23—H23	0.9500
Eu1—N3	2.555 (3)	C23—C24	1.364 (7)
Eu1—N5	2.573 (3)	C24—H24	0.9500
O1—C1	1.251 (5)	C24—C25	1.410 (9)
O2—C3	1.258 (5)	C25—H25	0.9500
O3—C18	1.266 (5)	C25—C26	1.339 (10)
O4—C20	1.261 (5)	C26—H26	0.9500
O5—C48	1.223 (6)	C26—C27	1.434 (9)
N1—N2	1.357 (5)	C27—C28	1.359 (9)
N1—C40	1.333 (5)	C28—H28	0.9500
N2—C38	1.339 (5)	C28—C29	1.393 (9)
N2—B1	1.549 (6)	C29—C30	1.411 (9)
N3—N4	1.359 (4)	C29—C34	1.455 (7)
N3—C41	1.330 (6)	C30—H30	0.9500
N4—C43	1.340 (6)	C30—C31	1.348 (11)
N4—B1	1.538 (6)	C31—H31	0.9500
N5—N6	1.346 (5)	C31—C32	1.422 (10)
N5—C35	1.326 (6)	C32—H32	0.9500
N6—C37	1.343 (6)	C32—C33	1.374 (8)
N6—B1	1.542 (7)	C33—H33	0.9500
N7—C48	1.312 (7)	C33—C34	1.407 (8)
N7—C49	1.452 (9)	C35—H35	0.9500
N7—C50	1.431 (10)	C35—C36	1.374 (9)
C1—C2	1.421 (5)	C36—H36	0.9500
C1—C45	1.507 (5)	C36—C37	1.380 (10)
C2—C3	1.413 (5)	C37—H37	0.9500
C2—C4	1.495 (5)	C38—H38	0.9500
C3—C44	1.522 (6)	C38—C39	1.374 (6)
C4—C5	1.409 (6)	C39—H39	0.9500
C4—C17	1.402 (6)	C39—C40	1.387 (5)
C5—C6	1.408 (7)	C40—H40	0.9500
C5—C10	1.445 (6)	C41—H41	0.9500
C6—H6	0.9500	C41—C42	1.383 (7)
C6—C7	1.370 (7)	C42—H42	0.9500
C7—H7	0.9500	C42—C43	1.374 (7)
C7—C8	1.427 (10)	C43—H43	0.9500
C8—H8	0.9500	C44—H44A	0.9800
C8—C9	1.335 (10)	C44—H44B	0.9800
C9—H9	0.9500	C44—H44C	0.9800

C9—C10	1.423 (9)	C45—H45A	0.9800
C10—C11	1.377 (9)	C45—H45B	0.9800
C11—H11	0.9500	C45—H45C	0.9800
C11—C12	1.372 (9)	C46—H46A	0.9800
C12—C13	1.430 (9)	C46—H46B	0.9800
C12—C17	1.436 (6)	C46—H46C	0.9800
C13—H13	0.9500	C47—H47A	0.9800
C13—C14	1.347 (11)	C47—H47B	0.9800
C14—H14	0.9500	C47—H47C	0.9800
C14—C15	1.409 (11)	C48—H48	0.9500
C15—H15	0.9500	C49—H49A	0.9800
C15—C16	1.366 (8)	C49—H49B	0.9800
C16—H16	0.9500	C49—H49C	0.9800
C16—C17	1.429 (7)	C50—H50A	0.9800
C18—C19	1.409 (5)	C50—H50B	0.9800
C18—C47	1.513 (5)	C50—H50C	0.9800
C19—C20	1.402 (5)	B1—H1	1.0000
C19—C21	1.512 (5)		
O1—Eu1—O5	75.01 (11)	C22—C21—C19	118.8 (4)
O1—Eu1—N1	145.99 (10)	C34—C21—C19	121.1 (4)
O1—Eu1—N3	142.63 (10)	C34—C21—C22	120.0 (4)
O1—Eu1—N5	118.84 (11)	C21—C22—C27	119.9 (5)
O2—Eu1—O1	70.86 (9)	C23—C22—C21	122.8 (4)
O2—Eu1—O3	145.67 (9)	C23—C22—C27	117.3 (5)
O2—Eu1—O4	86.42 (12)	C22—C23—H23	118.8
O2—Eu1—O5	109.01 (12)	C24—C23—C22	122.3 (5)
O2—Eu1—N1	140.38 (10)	C24—C23—H23	118.8
O2—Eu1—N3	79.35 (11)	C23—C24—H24	120.0
O2—Eu1—N5	72.80 (11)	C23—C24—C25	120.1 (7)
O3—Eu1—O1	79.81 (9)	C25—C24—H24	120.0
O3—Eu1—O5	79.12 (10)	C24—C25—H25	119.9
O3—Eu1—N1	73.13 (9)	C26—C25—C24	120.3 (6)
O3—Eu1—N3	117.69 (11)	C26—C25—H25	119.9
O3—Eu1—N5	139.36 (10)	C25—C26—H26	119.1
O4—Eu1—O1	80.32 (11)	C25—C26—C27	121.8 (5)
O4—Eu1—O3	71.10 (9)	C27—C26—H26	119.1
O4—Eu1—O5	144.11 (10)	C26—C27—C22	118.2 (6)
O4—Eu1—N1	109.05 (11)	C28—C27—C22	119.1 (5)
O4—Eu1—N3	75.70 (10)	C28—C27—C26	122.7 (5)
O4—Eu1—N5	143.07 (11)	C27—C28—H28	118.6
O5—Eu1—N1	79.92 (11)	C27—C28—C29	122.8 (4)
O5—Eu1—N3	137.76 (10)	C29—C28—H28	118.6
O5—Eu1—N5	72.66 (11)	C28—C29—C30	123.2 (6)
N3—Eu1—N1	70.18 (10)	C28—C29—C34	119.0 (5)
N3—Eu1—N5	70.74 (11)	C30—C29—C34	117.8 (6)
N5—Eu1—N1	73.60 (11)	C29—C30—H30	119.4
C1—O1—Eu1	137.5 (2)	C31—C30—C29	121.2 (6)

C3—O2—Eu1	139.3 (3)	C31—C30—H30	119.4
C18—O3—Eu1	135.7 (2)	C30—C31—H31	118.9
C20—O4—Eu1	135.2 (3)	C30—C31—C32	122.3 (6)
C48—O5—Eu1	134.9 (3)	C32—C31—H31	118.9
N2—N1—Eu1	125.2 (2)	C31—C32—H32	121.1
C40—N1—Eu1	128.1 (3)	C33—C32—C31	117.9 (7)
C40—N1—N2	105.9 (3)	C33—C32—H32	121.1
N1—N2—B1	121.4 (3)	C32—C33—H33	118.9
C38—N2—N1	110.1 (3)	C32—C33—C34	122.3 (6)
C38—N2—B1	128.4 (3)	C34—C33—H33	118.9
N4—N3—Eu1	125.2 (2)	C21—C34—C29	119.1 (5)
C41—N3—Eu1	128.2 (3)	C21—C34—C33	122.3 (4)
C41—N3—N4	106.1 (3)	C33—C34—C29	118.6 (5)
N3—N4—B1	122.4 (3)	N5—C35—H35	124.6
C43—N4—N3	109.8 (3)	N5—C35—C36	110.9 (6)
C43—N4—B1	127.7 (4)	C36—C35—H35	124.6
N6—N5—Eu1	125.4 (2)	C35—C36—H36	127.6
C35—N5—Eu1	126.3 (3)	C35—C36—C37	104.8 (5)
C35—N5—N6	106.6 (4)	C37—C36—H36	127.6
N5—N6—B1	121.6 (3)	N6—C37—C36	107.8 (5)
C37—N6—N5	109.9 (4)	N6—C37—H37	126.1
C37—N6—B1	128.4 (4)	C36—C37—H37	126.1
C48—N7—C49	119.4 (7)	N2—C38—H38	125.8
C48—N7—C50	122.5 (6)	N2—C38—C39	108.5 (4)
C50—N7—C49	118.0 (7)	C39—C38—H38	125.8
O1—C1—C2	125.6 (4)	C38—C39—H39	127.7
O1—C1—C45	116.1 (3)	C38—C39—C40	104.5 (4)
C2—C1—C45	118.2 (3)	C40—C39—H39	127.7
C1—C2—C4	120.3 (3)	N1—C40—C39	110.9 (4)
C3—C2—C1	120.5 (3)	N1—C40—H40	124.5
C3—C2—C4	119.2 (3)	C39—C40—H40	124.5
O2—C3—C2	124.9 (4)	N3—C41—H41	124.5
O2—C3—C44	116.1 (4)	N3—C41—C42	111.0 (4)
C2—C3—C44	119.1 (4)	C42—C41—H41	124.5
C5—C4—C2	120.4 (4)	C41—C42—H42	127.7
C17—C4—C2	120.1 (4)	C43—C42—C41	104.6 (4)
C17—C4—C5	119.5 (4)	C43—C42—H42	127.7
C4—C5—C10	118.9 (5)	N4—C43—C42	108.5 (4)
C6—C5—C4	123.2 (4)	N4—C43—H43	125.7
C6—C5—C10	117.9 (5)	C42—C43—H43	125.7
C5—C6—H6	118.8	C3—C44—H44A	109.5
C7—C6—C5	122.3 (5)	C3—C44—H44B	109.5
C7—C6—H6	118.8	C3—C44—H44C	109.5
C6—C7—H7	120.5	H44A—C44—H44B	109.5
C6—C7—C8	119.0 (7)	H44A—C44—H44C	109.5
C8—C7—H7	120.5	H44B—C44—H44C	109.5
C7—C8—H8	119.7	C1—C45—H45A	109.5
C9—C8—C7	120.7 (6)	C1—C45—H45B	109.5

C9—C8—H8	119.7	C1—C45—H45C	109.5
C8—C9—H9	118.9	H45A—C45—H45B	109.5
C8—C9—C10	122.1 (6)	H45A—C45—H45C	109.5
C10—C9—H9	118.9	H45B—C45—H45C	109.5
C9—C10—C5	118.0 (6)	C20—C46—H46A	109.5
C11—C10—C5	120.0 (5)	C20—C46—H46B	109.5
C11—C10—C9	122.0 (5)	C20—C46—H46C	109.5
C10—C11—H11	119.0	H46A—C46—H46B	109.5
C12—C11—C10	122.0 (4)	H46A—C46—H46C	109.5
C12—C11—H11	119.0	H46B—C46—H46C	109.5
C11—C12—C13	122.9 (5)	C18—C47—H47A	109.5
C11—C12—C17	119.0 (5)	C18—C47—H47B	109.5
C13—C12—C17	118.1 (6)	C18—C47—H47C	109.5
C12—C13—H13	118.9	H47A—C47—H47B	109.5
C14—C13—C12	122.2 (6)	H47A—C47—H47C	109.5
C14—C13—H13	118.9	H47B—C47—H47C	109.5
C13—C14—H14	120.1	O5—C48—N7	124.7 (6)
C13—C14—C15	119.7 (6)	O5—C48—H48	117.6
C15—C14—H14	120.1	N7—C48—H48	117.6
C14—C15—H15	119.5	N7—C49—H49A	109.5
C16—C15—C14	120.9 (7)	N7—C49—H49B	109.5
C16—C15—H15	119.5	N7—C49—H49C	109.5
C15—C16—H16	119.5	H49A—C49—H49B	109.5
C15—C16—C17	121.1 (6)	H49A—C49—H49C	109.5
C17—C16—H16	119.5	H49B—C49—H49C	109.5
C4—C17—C12	120.6 (5)	N7—C50—H50A	109.5
C4—C17—C16	121.5 (4)	N7—C50—H50B	109.5
C16—C17—C12	117.9 (5)	N7—C50—H50C	109.5
O3—C18—C19	124.9 (3)	H50A—C50—H50B	109.5
O3—C18—C47	115.2 (3)	H50A—C50—H50C	109.5
C19—C18—C47	120.0 (3)	H50B—C50—H50C	109.5
C18—C19—C21	118.2 (3)	N2—B1—H1	109.9
C20—C19—C18	122.0 (3)	N4—B1—N2	109.6 (3)
C20—C19—C21	119.8 (3)	N4—B1—N6	109.7 (3)
O4—C20—C19	125.1 (3)	N4—B1—H1	109.9
O4—C20—C46	115.7 (4)	N6—B1—N2	107.9 (4)
C19—C20—C46	119.3 (3)	N6—B1—H1	109.9