2 Nov 2006

Acta Cryst. (2004). C60, 000–000**A Eu-based Metal Organic Framework, poly[[tris(μ_4 -benzene-1,4-dicarboxylato)-bis(μ_2 -*N,N*-diethylformamide)dieuropium(III)]hydrate]**HENRIK F. CLAUSEN,^a JACOB OVERGAARD,^a RASMUS D. POULSEN,^a WOLFGANG MORGENROTH^b AND BO B. IVERSEN^a^a*Department of Chemistry, University of Aarhus, Langelandsgade 140, DK-8000 Aarhus C, Denmark, and* ^b*Deutsches Elektronen-Synchrotron, D3 beamline, Hasylab, Notkestraße 85, Hamburg D-22603, Germany. E-mail: bo@chem.au.dk***Abstract**

The crystal structure of the title compound, $[\text{Eu}_2(\text{C}_8\text{H}_4\text{O}_4)_3(\text{C}_5\text{H}_{11}\text{NO})_2 \cdot 0.7\text{H}_2\text{O}]_n$, consists of chains formed by Eu atoms intraconnected by the carboxylate groups of the benzene-1,4-dicarboxylate linker (BDC). The chains are interconnected by BDC linkers, consequently generating a three dimensional framework with large voids. The europium atoms coordinate to seven carboxylate O atoms and one solvent oxygen in a sterically constrained manner due to the carboxylate group rigidity, and this causes the coordination to be distorted dodecahedral. The ethyl groups of the solvent molecule are disordered in the void. The elongated Eu–O bond of the solvent indicates that it is loosely bound to the framework, and hence solvent exchange may be possible. In the void there is additionally one partly occupied disordered water molecule.

Comment

Metal Organic Frameworks (MOFs) are of great scientific interest (Kitahawa *et al.*, 2004; Lu, J. Y., 2003; O’Keeffe *et al.*, 2000). Their potential use in gas storage has enormous attention world wide. The main research activity in our group has focused on the magnetic properties of these compounds (Zhang *et al.*, 2005). The present structure is one in a series of MOFs which may combine interesting magnetic effects and potential gas storage due to the electron rich metal centers. An isostructural Gd-based compound was reported by Poulsen *et al.* (2005a).

Europium atoms are intraconnected by carboxylate groups of the deprotonated terephthalic acid generating chains of metal atoms. These chains are interconnected by the terephthalic acid molecules resulting in a three dimensional network. The intra-chain Eu–Eu-distance is alternate 4.034 (2) Å and 5.572 (4) Å, whereas the inter-chain distance is much larger (>9.6 Å). This could lead to a unique magnetic direction along the *c*-axis of the unit cell.

The short intra-chain distance has four bridging carboxylate groups and two direct μ -bridging O atoms (O12). The bridging atom has one short ($d_{\text{Eu}-\text{O}} = 2.4007(15)$ Å) and one long ($d_{\text{Eu}-\text{O}} = 2.7884(18)$ Å) bond to the Eu atoms. Not including the longer bridging bond, the bond average

from the carboxylate O atoms to the europium atom $\langle \text{Eu}-\text{O}(\text{carboxylate}) \rangle$ is 2.353 (2) Å. This bond average is smaller than the bond to the diethyl formamide molecule, $\langle \text{Eu}-\text{O}(\text{DEF}) \rangle = 2.436$ (6) Å, hence this molecule is more weakly bonded and could be a subject to solvent exchange. Due to the sterically constrained carboxylate groups, the coordination of the europium atoms are distorted dodecahedral.

Some degree of electron localization is observed in the carboxylate group bridging the long Eu–Eu distance, while the others are delocalized. A carboxylate group has a net charge of $-1 e^-$, and a formal electron count suggests that the Eu atom has a charge of +3, which is in agreement with synthesis conditions.

The voids of the network are occupied by disordered solvent molecules (53%/47%), which are directly bonded to the Eu atoms. The bonding of solvent to the framework metal center was previously reported in Mn-based systems (Poulsen *et al.*, 2004, 2005*b*).

A partially occupied water molecule (35%), which is disordered into two equivalent crystallographic positions, is also occupying the void. The large displacement parameter observed for the C19B could be due to hydrogen bonding to the partly occupied water molecule, O99.

0.

Experimental

The compound was prepared by adding a mixture of $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$ (1.0 mmol, $m=0.366\text{g}$) and 3 ml DEF to a mixture benzene dicarboxylic acid (1mmol, 0.166g), H_2BDC , and 7 ml of DEF in an autoclave. After heating at 120°C for 72 h white crystals suitable for single-crystal X-ray diffraction experiments were formed.

0.

Crystal data

$\text{C}_{17}\text{H}_{17}\text{EuNO}_7 \cdot 0.35$

H_2O

$M_r = 505.08$

Monoclinic

$C2/c$

$a = 18.010$ (7) Å

$b = 11.478$ (7) Å

$c = 18.743$ (12) Å

$\beta = 108.91$ (3)°

$V = 3665$ (4) Å³

$Z = 8$

$D_x = 1.831$ Mg m⁻³

D_m not measured

synchrotron radiation

$\lambda = 0.55000$ Å

Cell parameters from 57266 reflections

$\theta = 1.73\text{--}38.83^\circ$

$\mu = 1.626$ mm⁻¹

$T = 100$ (2) K

Rectuangular

White

$0.100 \times 0.100 \times 0.075$ mm

Data collection

Huber four-circle diffractometer	19344 reflections with
Phi-scans	$>2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.126$
424451 measured reflections	$\theta_{\text{max}} = 38.81^\circ$
22159 independent reflections	$h = 0 \rightarrow 40$
	$k = 0 \rightarrow 25$
	$l = -42 \rightarrow 39$

Refinement

Refinement on F^2	$(\Delta/\sigma)_{\text{max}} = 0.011$
$R[F^2 > 2\sigma(F^2)] = 0.0366$	$\Delta\rho_{\text{max}} = 3.467 \text{ e } \text{\AA}^{-3}$
$wR(F^2) = 0.0899$	$\Delta\rho_{\text{min}} = -3.257 \text{ e } \text{\AA}^{-3}$
$S = 1.052$	Extinction correction: <i>SHELXL</i>
22159 reflections	Extinction coefficient: 0.00453 (17)
288 parameters	Scattering factors from <i>International Tables</i>
H-atom parameters constrained	for <i>Crystallography</i> (Vol. C)
$w=1/[\sigma^2(F_o^2) + (0.0449P)^2 + 7.3908P]$	
where $P = (F_o^2 + 2F_c^2)/3$	

A correction for the oblique incidence of the X-ray beam through the detector has been made using a transmission factor of 0.37 for the MarCCD detector measured at a wavelength of 0.55 Å. H atoms were included in calculated positions and refined in a riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms besides the methyl groups where the value was $1.5U_{\text{eq}}(\text{C})$. The disorder in the DEF molecule has no overlapping positions, and the sum of two disordered occupancies was fixed to unity. Bonding to the framework limits the disorder in the DEF molecule and enables refinement of the anisotropic displacement parameters of all non-H atoms. The occupancy of the water molecule was refined to 35%, and due to disorder the two H atoms could not be located, but they are included in the formula.

Cell refinement: XDS-2004 (Kabsch, 1993). Data reduction: XDS-2004 (Kabsch, 1993). Program(s) used to solve structure: *SHELXS-97* (Sheldrick, 1997). Program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997). Molecular graphics: XShell (Version 4.02). Software used to prepare material for publication: *enCIFer v1.2* (CCDC, 2005).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: PREVIEW). Services for accessing these data are described at the back of the journal.

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Fig. 1: The asymmetric unit of the title compound. The disorder of the ethyl groups is shown with turquoise and red bonds (47%/53%). All ethyl H atoms except H19D have been removed for clarity. Thermal ellipsoids are shown with 50% probability level.

Fig. 2: The packing of the structure viewed along the *c*-axis of the unit cell. 0.

Supplementary data

The tables of data shown below are not normally printed in *Acta Cryst. Section C* but the data will be available electronically *via* the online contents pages at

<http://journals.iucr.org/c/journalhomepage.html>

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$)

$$U_{\text{eq}} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i \cdot \mathbf{a}_j.$$

	Occupancy	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
Eu1	1	0.498091 (3)	0.058967 (4)	0.898036 (3)	0.00696 (1)
O1	1	0.40982 (7)	0.05628 (11)	0.77564 (6)	0.01829 (19)
O2	1	0.58662 (5)	0.01120 (9)	0.83855 (5)	0.01167 (11)
O8	1	0.56978 (8)	0.17803 (12)	0.99946 (6)	0.0222 (2)
O9	1	0.42636 (12)	−0.11407 (17)	0.88661 (7)	0.0408 (5)
O11	1	0.39304 (7)	0.18172 (11)	0.90617 (6)	0.01712 (16)
O12	1	0.42060 (7)	0.06532 (11)	1.00488 (8)	0.0209 (2)
O15	1	0.52735 (8)	0.24314 (10)	0.84810 (7)	0.01913 (17)
N15	1	0.55747 (17)	0.43506 (14)	0.86723 (17)	0.0381 (5)
C1	1	0.38204 (6)	0.05873 (10)	0.70580 (6)	0.01068 (13)
C2	1	0.80553 (7)	0.37928 (11)	1.17100 (6)	0.01217 (14)
C3	1	0.77018 (9)	0.32070 (15)	1.21686 (7)	0.0185 (2)
H3	1	0.7924	0.3242	1.2690	0.022
C4	1	0.70182 (12)	0.25721 (18)	1.18462 (7)	0.0256 (4)
H4	1	0.6785	0.2180	1.2152	0.031
C5	1	0.66815 (11)	0.25224 (15)	1.10620 (7)	0.0222 (3)
C6	1	0.70235 (9)	0.31309 (13)	1.06052 (7)	0.0182 (2)
H6	1	0.6791	0.3116	1.0084	0.022
C7	1	0.77102 (8)	0.37592 (13)	1.09267 (6)	0.01507 (18)
H7	1	0.7940	0.4158	1.0620	0.018
C8	1	0.59804 (13)	0.17659 (17)	1.07025 (8)	0.0267 (4)
C11	1	0.37941 (7)	0.14514 (13)	0.96395 (8)	0.01517 (18)
C12	1	0.31243 (8)	0.19848 (13)	0.98321 (8)	0.01555 (19)
C13	1	0.30288 (9)	0.17871 (14)	1.05310 (8)	0.0187 (2)
H13	1	0.3381	0.1314	1.0885	0.022
C14	1	0.25960 (9)	0.26990 (15)	0.93044 (8)	0.0204 (3)
H14	1	0.2662	0.2832	0.8839	0.024
C15	1	0.5187 (2)	0.33910 (18)	0.8711 (2)	0.0492 (9)
H15	1	0.4804	0.3459	0.8942	0.059
C16A	0.475 (3)	0.6342 (3)	0.4262 (4)	0.8584 (4)	0.0350 (10)
H16A	0.475 (3)	0.6457	0.3446	0.8534	0.042
H16B	0.475 (3)	0.6731	0.4555	0.9038	0.042
C18A	0.475 (3)	0.6420 (7)	0.4906 (12)	0.7926 (7)	0.086 (4)
H18A	0.475 (3)	0.6102	0.4539	0.7469	0.129
H18B	0.475 (3)	0.6959	0.4899	0.7944	0.129
H18C	0.475 (3)	0.6250	0.5696	0.7939	0.129
C16B	0.525 (3)	0.6014 (3)	0.4414 (3)	0.8133 (3)	0.0299 (8)
H16C	0.525 (3)	0.5774	0.5005	0.7760	0.036
H16D	0.525 (3)	0.5959	0.3674	0.7871	0.036
C18B	0.525 (3)	0.6870 (4)	0.4684 (8)	0.8469 (6)	0.060 (2)
H18D	0.525 (3)	0.6934	0.5436	0.8706	0.089
H18E	0.525 (3)	0.7108	0.4686	0.8079	0.089
H18F	0.525 (3)	0.7118	0.4103	0.8838	0.089
C17A	0.475 (3)	0.5233 (3)	0.5452 (3)	0.8816 (3)	0.0303 (9)
H17A	0.475 (3)	0.4677	0.5358	0.8740	0.036
H17B	0.475 (3)	0.5298	0.6057	0.8480	0.036
C19A	0.475 (3)	0.5668 (4)	0.5764 (6)	0.9623 (4)	0.052 (2)
H19A	0.475 (3)	0.5619	0.5140	0.9946	0.078
H19B	0.475 (3)	0.5450	0.6463	0.9754	0.078
H19C	0.475 (3)	0.6212	0.5887	0.9684	0.078
C17B	0.525 (3)	0.5679 (4)	0.5393 (4)	0.9200 (5)	0.0542 (19)
H17C	0.525 (3)	0.5557	0.5166	0.9648	0.065
H17D	0.525 (3)	0.6220	0.5653	0.9355	0.065
C19B	0.525 (3)	0.5152 (6)	0.6364 (6)	0.8812 (8)	0.113 (5)
H19D	0.525 (3)	0.5272	0.6585	0.8368	0.169
H19E	0.525 (3)	0.5228	0.7019	0.9146	0.169
H19F	0.525 (3)	0.4615	0.6112	0.8672	0.169

O99 0.350 (8) 0.4752 (5) 0.7751 (5) 0.7560 (4) 0.047 (2)

Table S2. *Anisotropic displacement parameters* ($\text{\AA}^2$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu1	0.00569 (2)	0.00944 (2)	0.00551 (2)	0.00041 (1)	0.00151 (1)	−0.00021 (1)
O1	0.0123 (3)	0.0333 (6)	0.0073 (3)	0.0056 (3)	0.0004 (2)	−0.0010 (3)
O2	0.0094 (2)	0.0166 (3)	0.0099 (2)	0.0020 (2)	0.0044 (2)	0.0015 (2)
O8	0.0301 (5)	0.0240 (5)	0.0087 (3)	−0.0159 (4)	0.0012 (3)	−0.0021 (3)
O9	0.0594 (11)	0.0475 (9)	0.0106 (4)	−0.0440 (9)	0.0045 (5)	−0.0021 (4)
O11	0.0174 (4)	0.0221 (4)	0.0154 (3)	0.0096 (3)	0.0102 (3)	0.0065 (3)
O12	0.0170 (4)	0.0248 (5)	0.0248 (5)	0.0137 (3)	0.0121 (4)	0.0136 (4)
O15	0.0264 (5)	0.0158 (4)	0.0162 (4)	−0.0012 (3)	0.0082 (4)	0.0027 (3)
N15	0.0541 (14)	0.0132 (5)	0.0595 (15)	0.0017 (6)	0.0359 (13)	0.0027 (6)
C1	0.0083 (3)	0.0158 (4)	0.0074 (3)	−0.0003 (3)	0.0017 (2)	−0.0005 (3)
C2	0.0135 (4)	0.0150 (4)	0.0071 (3)	−0.0028 (3)	0.0020 (3)	−0.0006 (3)
C3	0.0218 (5)	0.0251 (6)	0.0072 (3)	−0.0123 (4)	0.0027 (3)	−0.0010 (3)
C4	0.0331 (8)	0.0334 (8)	0.0080 (4)	−0.0228 (7)	0.0033 (4)	−0.0012 (4)
C5	0.0306 (7)	0.0247 (6)	0.0083 (3)	−0.0182 (5)	0.0021 (4)	−0.0021 (4)
C6	0.0235 (5)	0.0211 (5)	0.0072 (3)	−0.0113 (4)	0.0012 (3)	−0.0009 (3)
C7	0.0171 (4)	0.0193 (5)	0.0076 (3)	−0.0062 (4)	0.0024 (3)	−0.0001 (3)
C8	0.0383 (8)	0.0293 (7)	0.0089 (4)	−0.0247 (7)	0.0025 (4)	−0.0021 (4)
C11	0.0132 (4)	0.0191 (5)	0.0164 (4)	0.0092 (3)	0.0092 (3)	0.0069 (3)
C12	0.0139 (4)	0.0200 (5)	0.0161 (4)	0.0099 (3)	0.0094 (3)	0.0082 (4)
C13	0.0177 (5)	0.0249 (6)	0.0168 (4)	0.0139 (4)	0.0103 (4)	0.0105 (4)
C14	0.0198 (5)	0.0288 (6)	0.0171 (5)	0.0160 (5)	0.0122 (4)	0.0118 (4)
C15	0.0695 (19)	0.0140 (6)	0.093 (2)	0.0074 (8)	0.066 (2)	0.0081 (9)
C16A	0.042 (3)	0.0231 (17)	0.046 (3)	−0.0012 (16)	0.023 (2)	0.0059 (17)
C18A	0.084 (7)	0.101 (9)	0.096 (8)	0.027 (6)	0.062 (7)	0.064 (7)
C16B	0.0315 (18)	0.0223 (13)	0.037 (2)	−0.0065 (11)	0.0122 (16)	0.0090 (12)
C18B	0.034 (3)	0.058 (4)	0.082 (6)	−0.008 (3)	0.012 (3)	0.005 (4)
C17A	0.033 (2)	0.0117 (11)	0.045 (3)	0.0007 (11)	0.0108 (19)	−0.0031 (12)
C19A	0.046 (3)	0.035 (3)	0.070 (5)	−0.004 (2)	0.012 (3)	−0.032 (3)
C17B	0.054 (4)	0.0226 (17)	0.089 (6)	−0.009 (2)	0.027 (4)	−0.022 (3)
C19B	0.059 (4)	0.040 (3)	0.183 (12)	0.020 (3)	−0.039 (6)	−0.055 (5)
O99	0.083 (6)	0.027 (2)	0.039 (3)	−0.005 (3)	0.030 (3)	0.003 (2)

Table S3. *Geometric parameters* ($\text{\AA}$, $^\circ$)

Eu1—O2	2.2888 (12)	C7—H7	0.9300
Eu1—O1	2.3295 (18)	C11—C12	1.4976 (16)
Eu1—O9	2.3410 (17)	C12—C13	1.3940 (19)
Eu1—O8	2.3574 (15)	C12—C14	1.3948 (18)
Eu1—O12 ⁱ	2.4007 (15)	C13—C14 ^{iv}	1.3907 (18)
Eu1—O11	2.4031 (12)	C13—H13	0.9300
Eu1—O15	2.4376 (16)	C14—H14	0.9300
Eu1—O12	2.7884 (18)	C15—H15	0.9300
Eu1—Eu1 ⁱ	4.034 (2)	C16A—C18A	1.483 (7)
O1—C1	1.2410 (17)	C16A—H16A	0.9700
O2—C1 ⁱⁱ	1.2694 (15)	C16A—H16B	0.9700
O8—C8	1.2577 (19)	C18A—H18A	0.9600
O9—C8 ⁱ	1.262 (2)	C18A—H18B	0.9600
O11—C11	1.2576 (17)	C18A—H18C	0.9600
O12—C11	1.2686 (16)	C16B—C18B	1.497 (6)
O15—C15	1.211 (3)	C16B—H16C	0.9700
N15—C15	1.318 (3)	C16B—H16D	0.9700
N15—C16A	1.448 (5)	C18B—H18D	0.9600
N15—C17A	1.469 (4)	C18B—H18E	0.9600
N15—C16B	1.473 (5)	C18B—H18F	0.9600
N15—C17B	1.524 (5)	C17A—C19A	1.503 (7)
C1—C2 ⁱⁱⁱ	1.4991 (17)	C17A—H17A	0.9700
C2—C3	1.3968 (18)	C17A—H17B	0.9700
C2—C7	1.3971 (18)	C19A—H19A	0.9600
C3—C4	1.389 (2)	C19A—H19B	0.9600
C3—H3	0.9300	C19A—H19C	0.9600
C4—C5	1.398 (2)	C17B—C19B	1.491 (7)
C4—H4	0.9300	C17B—H17C	0.9700
C5—C6	1.394 (2)	C17B—H17D	0.9700
C5—C8	1.500 (2)	C19B—H19D	0.9600
C6—C7	1.3891 (19)	C19B—H19E	0.9600
C6—H6	0.9300	C19B—H19F	0.9600
		O99—O99 ⁱⁱ	0.987 (15)

O2—Eu1—O1	82.99 (5)	C3—C2—C7	119.81 (11)
O2—Eu1—O9	101.72 (7)	C3—C2—C1 ^v	119.91 (10)
O1—Eu1—O9	73.65 (5)	C7—C2—C1 ^v	120.23 (11)
O2—Eu1—O8	104.23 (6)	C4—C3—C2	120.09 (12)
O1—Eu1—O8	145.32 (5)	C4—C3—H3	120.0
O9—Eu1—O8	135.02 (5)	C2—C3—H3	120.0
O2—Eu1—O12 ⁱ	82.92 (5)	C3—C4—C5	120.01 (13)
O1—Eu1—O12 ⁱ	142.42 (5)	C3—C4—H4	120.0
O9—Eu1—O12 ⁱ	75.41 (7)	C5—C4—H4	120.0
O8—Eu1—O12 ⁱ	72.13 (7)	C6—C5—C4	119.87 (13)
O2—Eu1—O11	149.14 (4)	C6—C5—C8	119.30 (12)
O1—Eu1—O11	76.72 (5)	C4—C5—C8	120.74 (13)
O9—Eu1—O11	94.63 (8)	C7—C6—C5	120.16 (12)
O8—Eu1—O11	81.12 (6)	C7—C6—H6	119.9
O12 ⁱ —Eu1—O11	126.85 (5)	C5—C6—H6	119.9
O2—Eu1—O15	75.48 (5)	C6—C7—C2	120.03 (12)
O1—Eu1—O15	78.28 (5)	C6—C7—H7	120.0
O9—Eu1—O15	151.91 (5)	C2—C7—H7	120.0
O8—Eu1—O15	71.14 (6)	O8—C8—O9 ⁱ	125.27 (14)
O12 ⁱ —Eu1—O15	130.67 (5)	O8—C8—C5	117.40 (13)
O11—Eu1—O15	77.79 (5)	O9 ⁱ —C8—C5	117.29 (13)
O2—Eu1—O12	161.08 (3)	O11—C11—O12	121.52 (11)
O1—Eu1—O12	111.53 (6)	O11—C11—C12	117.92 (11)
O9—Eu1—O12	72.42 (6)	O12—C11—C12	120.56 (12)
O8—Eu1—O12	71.12 (6)	O11—C11—Eu1	51.98 (7)
O12 ⁱ —Eu1—O12	78.20 (5)	O12—C11—Eu1	69.62 (8)
O11—Eu1—O12	49.57 (4)	C12—C11—Eu1	169.41 (9)
O15—Eu1—O12	118.29 (4)	C13—C12—C14	119.90 (11)
O2—Eu1—C11	173.39 (3)	C13—C12—C11	120.95 (11)
O1—Eu1—C11	93.48 (6)	C14—C12—C11	119.15 (11)
O9—Eu1—C11	82.54 (7)	C14 ^{iv} —C13—C12	119.64 (11)
O8—Eu1—C11	75.57 (6)	C14 ^{iv} —C13—H13	120.2
O12 ⁱ —Eu1—C11	103.15 (5)	C12—C13—H13	120.2
O11—Eu1—C11	24.35 (4)	C13 ^{iv} —C14—C12	120.46 (12)
O15—Eu1—C11	98.37 (5)	C13 ^{iv} —C14—H14	119.8
O12—Eu1—C11	25.24 (3)	C12—C14—H14	119.8
O2—Eu1—Eu1 ⁱ	125.49 (4)	O15—C15—N15	127.5 (2)
O1—Eu1—Eu1 ⁱ	136.48 (4)	O15—C15—H15	116.3
O9—Eu1—Eu1 ⁱ	68.99 (4)	N15—C15—H15	116.3
O8—Eu1—Eu1 ⁱ	66.04 (5)	N15—C16A—C18A	114.3 (6)
O12 ⁱ —Eu1—Eu1 ⁱ	42.57 (4)	N15—C16A—H16A	108.7
O11—Eu1—Eu1 ⁱ	84.76 (4)	C18A—C16A—H16A	108.7
O15—Eu1—Eu1 ⁱ	135.67 (3)	N15—C16A—H16B	108.7
O12—Eu1—Eu1 ⁱ	35.63 (3)	C18A—C16A—H16B	108.7
C11—Eu1—Eu1 ⁱ	60.67 (4)	H16A—C16A—H16B	107.6
C1—O1—Eu1	162.10 (10)	C16A—C18A—H18A	109.5
C1 ⁱⁱ —O2—Eu1	138.06 (9)	C16A—C18A—H18B	109.5
C8—O8—Eu1	140.50 (11)	H18A—C18A—H18B	109.5
C8 ⁱ —O9—Eu1	136.09 (11)	C16A—C18A—H18C	109.5
C11—O11—Eu1	103.67 (8)	H18B—C18A—H18C	109.5
C11—O12—Eu1 ⁱ	168.82 (13)	N15—C16B—C18B	115.5 (5)
C11—O12—Eu1	85.14 (9)	N15—C16B—H16C	108.4
Eu1 ⁱ —O12—Eu1	101.80 (5)	C18B—C16B—H16C	108.4
C15—O15—Eu1	125.67 (15)	N15—C16B—H16D	108.4
C15—N15—C16A	119.3 (3)	C18B—C16B—H16D	108.4
C15—N15—C17A	116.6 (3)	H16C—C16B—H16D	107.5
C16A—N15—C17A	123.6 (3)	N15—C17A—C19A	106.1 (4)
C15—N15—C16B	119.4 (2)	N15—C17A—H17A	110.5
C17A—N15—C16B	115.7 (3)	C19A—C17A—H17A	110.5
C15—N15—C17B	125.2 (4)	N15—C17A—H17B	110.5
C16A—N15—C17B	102.0 (4)	C19A—C17A—H17B	108.7
C16B—N15—C17B	115.2 (4)	C19B—C17B—N15	110.2 (6)
O1—C1—O2 ⁱⁱ	124.61 (12)	C19B—C17B—H17C	109.6
O1—C1—C2 ⁱⁱⁱ	117.99 (11)	N15—C17B—H17C	109.6
O2 ⁱⁱ —C1—C2 ⁱⁱⁱ	117.40 (10)	C19B—C17B—H17D	109.6
		N15—C17B—H17D	109.6
		H17C—C17B—H17D	108.1
O2—Eu1—O1—C1	−20.5 (3)	O9—Eu1—O1—C1	−124.9 (3)

O8—Eu1—O1—C1	84.5 (3)	O12—Eu1—O15—C15	8.3 (3)
O12 ⁱ —Eu1—O1—C1	−89.2 (3)	C11—Eu1—O15—C15	24.7 (3)
O11—Eu1—O1—C1	136.1 (3)	Eu1 ⁱ —Eu1—O15—C15	−31.3 (3)
O15—Eu1—O1—C1	56.1 (3)	Eu1—O1—C1—O2 ⁱⁱ	39.1 (4)
O12—Eu1—O1—C1	172.1 (3)	Eu1—O1—C1—C2 ⁱⁱⁱ	−141.8 (3)
C11—Eu1—O1—C1	153.9 (3)	C7—C2—C3—C4	1.4 (3)
Eu1 ⁱ —Eu1—O1—C1	−156.5 (3)	C1 ^v —C2—C3—C4	−176.05 (17)
O1—Eu1—O2—C1 ⁱⁱ	68.61 (12)	C2—C3—C4—C5	−0.2 (3)
O9—Eu1—O2—C1 ⁱⁱ	140.24 (12)	C3—C4—C5—C6	−1.4 (3)
O8—Eu1—O2—C1 ⁱⁱ	−76.84 (13)	C3—C4—C5—C8	175.1 (2)
O12 ⁱ —Eu1—O2—C1 ⁱⁱ	−146.32 (12)	C4—C5—C6—C7	1.8 (3)
O11—Eu1—O2—C1 ⁱⁱ	19.70 (16)	C8—C5—C6—C7	−174.71 (18)
O15—Eu1—O2—C1 ⁱⁱ	−11.05 (12)	C5—C6—C7—C2	−0.7 (3)
O12—Eu1—O2—C1 ⁱⁱ	−150.00 (13)	C3—C2—C7—C6	−0.9 (2)
Eu1 ⁱ —Eu1—O2—C1 ⁱⁱ	−147.33 (10)	C1 ^v —C2—C7—C6	176.51 (14)
O2—Eu1—O8—C8	−110.2 (2)	Eu1—O8—C8—O9 ⁱ	−24.6 (4)
O1—Eu1—O8—C8	151.4 (2)	Eu1—O8—C8—C5	153.16 (16)
O9—Eu1—O8—C8	13.1 (3)	C6—C5—C8—O8	−4.9 (3)
O12 ⁱ —Eu1—O8—C8	−32.7 (2)	C4—C5—C8—O8	178.6 (2)
O11—Eu1—O8—C8	100.8 (2)	C6—C5—C8—O9 ⁱ	173.1 (2)
O15—Eu1—O8—C8	−179.2 (3)	C4—C5—C8—O9 ⁱ	−3.4 (4)
O12—Eu1—O8—C8	50.6 (2)	Eu1—O11—C11—O12	3.61 (19)
C11—Eu1—O8—C8	76.6 (2)	Eu1—O11—C11—C12	−176.16 (12)
Eu1 ⁱ —Eu1—O8—C8	12.6 (2)	Eu1 ⁱ —O12—C11—O11	125.9 (5)
O2—Eu1—O9—C8 ⁱ	134.0 (3)	Eu1—O12—C11—O11	−3.03 (16)
O1—Eu1—O9—C8 ⁱ	−147.0 (3)	Eu1 ⁱ —O12—C11—C12	−54.4 (6)
O8—Eu1—O9—C8 ⁱ	9.8 (3)	Eu1—O12—C11—C12	176.73 (14)
O12 ⁱ —Eu1—O9—C8 ⁱ	54.6 (3)	Eu1 ⁱ —O12—C11—Eu1	128.9 (6)
O11—Eu1—O9—C8 ⁱ	−72.3 (3)	O1—Eu1—C11—O11	−46.15 (11)
O15—Eu1—O9—C8 ⁱ	−144.9 (2)	O9—Eu1—C11—O11	−119.14 (12)
O12—Eu1—O9—C8 ⁱ	−27.4 (3)	O8—Eu1—C11—O11	100.47 (12)
C11—Eu1—O9—C8 ⁱ	−51.1 (3)	O12 ⁱ —Eu1—C11—O11	167.80 (11)
Eu1 ⁱ —Eu1—O9—C8 ⁱ	10.3 (3)	O15—Eu1—C11—O11	32.50 (11)
O2—Eu1—O11—C11	−177.47 (9)	O12—Eu1—C11—O11	176.72 (17)
O1—Eu1—O11—C11	132.31 (12)	Eu1 ⁱ —Eu1—C11—O11	170.81 (12)
O9—Eu1—O11—C11	60.32 (11)	O1—Eu1—C11—O12	137.13 (11)
O8—Eu1—O11—C11	−74.56 (12)	O9—Eu1—C11—O12	64.14 (12)
O12 ⁱ —Eu1—O11—C11	−14.90 (13)	O8—Eu1—C11—O12	−76.25 (11)
O15—Eu1—O11—C11	−147.05 (11)	O12 ⁱ —Eu1—C11—O12	−8.92 (14)
O12—Eu1—O11—C11	−1.84 (10)	O11—Eu1—C11—O12	−176.72 (18)
Eu1 ⁱ —Eu1—O11—C11	−8.04 (10)	O15—Eu1—C11—O12	−144.22 (11)
O2—Eu1—O12—C11	174.86 (11)	Eu1 ⁱ —Eu1—C11—O12	−5.91 (9)
O1—Eu1—O12—C11	−46.88 (12)	O1—Eu1—C11—C12	−27.4 (6)
O9—Eu1—O12—C11	−110.63 (13)	O9—Eu1—C11—C12	−100.4 (6)
O8—Eu1—O12—C11	96.19 (12)	O8—Eu1—C11—C12	119.2 (6)
O12 ⁱ —Eu1—O12—C11	171.13 (14)	O12 ⁱ —Eu1—C11—C12	−173.4 (6)
O11—Eu1—O12—C11	1.78 (10)	O11—Eu1—C11—C12	18.8 (6)
O15—Eu1—O12—C11	41.07 (12)	O15—Eu1—C11—C12	51.3 (6)
Eu1 ⁱ —Eu1—O12—C11	171.13 (14)	O12—Eu1—C11—C12	−164.5 (7)
O2—Eu1—O12—Eu1 ⁱ	3.73 (16)	Eu1 ⁱ —Eu1—C11—C12	−170.4 (6)
O1—Eu1—O12—Eu1 ⁱ	141.99 (6)	O11—C11—C12—C13	−167.81 (16)
O9—Eu1—O12—Eu1 ⁱ	78.24 (8)	O12—C11—C12—C13	12.4 (3)
O8—Eu1—O12—Eu1 ⁱ	−74.94 (8)	Eu1—C11—C12—C13	175.5 (5)
O12 ⁱ —Eu1—O12—Eu1 ⁱ	0.0	O11—C11—C12—C14	11.5 (2)
O11—Eu1—O12—Eu1 ⁱ	−169.35 (8)	O12—C11—C12—C14	−168.30 (17)
O15—Eu1—O12—Eu1 ⁱ	−130.06 (5)	Eu1—C11—C12—C14	−5.2 (7)
C11—Eu1—O12—Eu1 ⁱ	−171.13 (14)	C14—C12—C13—C14 ^{iv}	0.3 (3)
O2—Eu1—O15—C15	−157.7 (3)	C11—C12—C13—C14 ^{iv}	179.55 (17)
O1—Eu1—O15—C15	116.6 (3)	C13—C12—C14—C13 ^{iv}	−0.3 (3)
O9—Eu1—O15—C15	114.6 (3)	C11—C12—C14—C13 ^{iv}	−179.56 (17)
O8—Eu1—O15—C15	−46.8 (3)	Eu1—O15—C15—N15	153.1 (3)
O12 ⁱ —Eu1—O15—C15	−90.7 (3)	C16A—N15—C15—O15	−22.3 (7)
O11—Eu1—O15—C15	37.9 (3)	C17A—N15—C15—O15	165.0 (4)
		C16B—N15—C15—O15	18.0 (6)
		C17B—N15—C15—O15	−155.7 (5)
		C15—N15—C16A—C18A	125.0 (8)

C17A—N15—C16A—C18A	−62.9 (10)	C16A—N15—C17A—C19A	−73.5 (6)
C16B—N15—C16A—C18A	24.7 (8)	C16B—N15—C17A—C19A	−113.0 (5)
C17B—N15—C16A—C18A	−92.4 (9)	C17B—N15—C17A—C19A	−15.3 (7)
C15—N15—C16B—C18B	−123.1 (5)	C15—N15—C17B—C19B	−104.2 (8)
C16A—N15—C16B—C18B	−23.0 (6)	C16A—N15—C17B—C19B	116.2 (8)
C17A—N15—C16B—C18B	89.5 (6)	C17A—N15—C17B—C19B	−17.4 (8)
C17B—N15—C16B—C18B	51.2 (6)	C16B—N15—C17B—C19B	81.9 (9)
C15—N15—C17A—C19A	98.8 (6)		

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