

[μ -N,N'-Bis(2-oxidobenzylidene)-1,2-ethanediamine](methanol)trinitrato-copper(II)europium(III)

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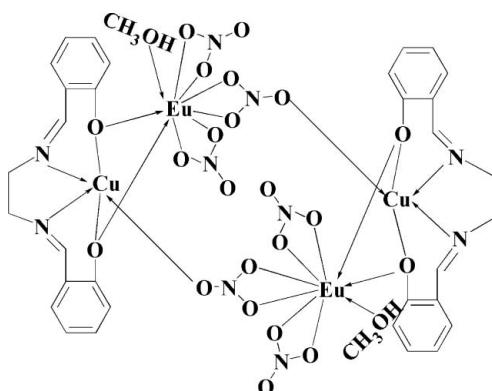
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.004$ Å; some non-H atoms missing; disorder in main residue; R factor = 0.021; wR factor = 0.047; data-to-parameter ratio = 15.1.

The title complex (systematic name: {2,2'-(ethane-1,2-diyl-bis(nitrilomethylidyne)]diphenolato-1κ⁴O¹,O^{1'},O⁶,O^{6'}:2κ⁴O¹,N,N',O^{1'}} (methanol-1κO)trinitrato-1κ⁶O,O'-copper(II)europium(III)), [CuEu(C₁₆H₁₄N₂O₂)(NO₃)₃(CH₃OH)], is a heterodinuclear 3d-4f metal Schiff base dimer. The Cu^{II} ion is five-coordinated by two O atoms, two N atoms of the deprotonated Schiff base and one nitrate O atom from a neighboring dinuclear unit, giving rise to a square-pyramidal geometry, whereas the Eu^{III} ion is nine-coordinated by six O atoms from nitrate groups, two O atoms from the deprotonated Schiff base and one O atom from methanol. The ethylene link is disordered over two positions with a site occupancy ratio of ca 3:1. The crystal structure involves O—H···O hydrogen bonds.

Related literature

See Kahn *et al.* (2000) for a similar copper–lanthanum complex of the same Schiff base.



Experimental

Crystal data

[CuEu(C ₁₆ H ₁₄ N ₂ O ₂)(NO ₃) ₃ ·(CH ₃ OH)]	$\beta = 102.451$ (12)°
$M_r = 699.87$	$V = 2277.6$ (12) Å ³
Monoclinic, $P2_1/c$	$Z = 4$
$a = 12.223$ (4) Å	Mo $K\alpha$ radiation
$b = 10.363$ (3) Å	$\mu = 3.74$ mm ⁻¹
$c = 18.414$ (5) Å	$T = 296$ (2) K

$0.33 \times 0.20 \times 0.19$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer	21558 measured reflections
Absorption correction: multi-scan (<i>ABSCOR</i> ; Higashi, 1995)	5201 independent reflections
$T_{\min} = 0.376$, $T_{\max} = 0.543$	4693 reflections with $I > 2\sigma(I)$
(expected range = 0.341–0.492)	$R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$	2 restraints
$wR(F^2) = 0.047$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\max} = 0.31$ e Å ⁻³
5201 reflections	$\Delta\rho_{\min} = -0.59$ e Å ⁻³
345 parameters	

Table 1
Selected bond lengths (Å).

Cu2—N2	1.918 (2)	Eu1—O4	2.455 (2)
Cu2—N1	1.925 (2)	Eu1—O7	2.4643 (19)
Cu2—O2	1.9301 (18)	Eu1—O6	2.476 (2)
Cu2—O1	1.9382 (17)	Eu1—O10	2.486 (2)
Cu2—O8	2.557 (19)	Eu1—O9	2.503 (2)
Eu1—O2	2.3589 (18)	Eu1—O12	2.5050 (19)
Eu1—O1	2.3662 (17)		
Eu1—O3	2.4474 (19)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H18···O12 ⁱ	0.85	2.04	2.886 (3)	174

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystaLStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2297).

metal-organic compounds

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[μ -N,N'-Bis(2-oxidobenzylidene)-1,2-ethanediamine](methanol)trinitratocopper(II)europium(III)

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Comment

As shown in Fig. 1, the tetradeятate Schiff base ligand links Cu and Eu atoms into a dinuclear complex through two phenolate O atoms. The Eu^{III} centre in (I) is nine-coordinated by two O atoms from the ligand, six O atoms from three nitrate and one O atoms from the methanol, which is similar with the bonding reported for another copper-lanthanum complex of the same ligand (Kahn *et al.*, 2000). The Cu^{II} center is five-coordinate by two N atoms, two O atoms from the ligand and one nitrato oxygen of neighboring dinuclear unit in a square-pyramidal geometry.

Experimental

The title complex was obtained by the treatment of copper(II) acetate monohydrate with the Schiff base in water/methanol (1:3). The first two reactants were stirred for 2 h, and the mixture was stirred for another 3 h after the addition of europium (III) nitrate hexahydrate. The reaction mixture was filtered; diethyl ether was allowed to diffuse slowly into the solution of the filtrate. Single crystals were obtained after several days. Analysis calculated for C₁₇H₁₇Cu₁Eu₁N₅O₁₂: C 29.22, H 2.45, N 10.02%; found: C 29.38, H 2.38, N 10.00%.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C), C—H = 0.97 Å (methylene C), and with $U_{\text{iso}}(\text{H}) = 1.2\text{U}_{\text{eq}}(\text{C})$ or C—H = 0.96 Å (methyl C) and with $U_{\text{iso}}(\text{H}) = 1.5\text{U}_{\text{eq}}(\text{C})$. The H atoms of hydroxy were initially located in a difference Fourier map but they were treated as riding on their parent atoms with O—H=0.85 Å, $U_{\text{iso}}(\text{H}) = 1.5\text{U}_{\text{eq}}(\text{O})$. In complex (I), the diaminopropane is disordered and was refined with a split model over two positions, and with an occupancy of 0.72 (2) for C8, C9, and 0.28 (2) for C8', C9'.

Figures

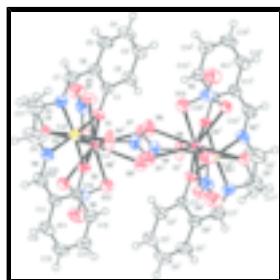


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. Disordered atoms (C8', C9') have been omitted for clarity.

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{2,2¹-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- 1κ⁴O¹,O^{1'},O⁶,O^{6'}: 2κ⁴O¹,N,N',O^{1'}}(methanol-1κO)trinitrato-1κ⁶O,O'-copper(II)europium(III)

Crystal data

[CuEu(C ₁₆ H ₁₄ N ₂ O ₂)(NO ₃) ₃ (CH ₄ O)]	$F_{000} = 1372$
$M_r = 699.87$	$D_x = 2.041 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 12.223 (4) \text{ \AA}$	Cell parameters from 18713 reflections
$b = 10.363 (3) \text{ \AA}$	$\theta = 6.0\text{--}54.9^\circ$
$c = 18.414 (5) \text{ \AA}$	$\mu = 3.74 \text{ mm}^{-1}$
$\beta = 102.451 (12)^\circ$	$T = 296 (2) \text{ K}$
$V = 2277.6 (12) \text{ \AA}^3$	Block, black
$Z = 4$	$0.33 \times 0.20 \times 0.19 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID diffractometer	5201 independent reflections
Radiation source: fine-focus sealed tube	4693 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.030$
Detector resolution: 10.000 pixels mm ⁻¹	$\theta_{\text{max}} = 27.5^\circ$
$T = 296(2) \text{ K}$	$\theta_{\text{min}} = 3.0^\circ$
ω scans	$h = -15\text{--}15$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -13\text{--}13$
$T_{\text{min}} = 0.376$, $T_{\text{max}} = 0.543$	$l = -23\text{--}22$
21558 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.021$	H-atom parameters constrained
$wR(F^2) = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0142P)^2 + 1.9917P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\text{max}} = 0.003$
5201 reflections	$\Delta\rho_{\text{max}} = 0.31 \text{ e \AA}^{-3}$
345 parameters	$\Delta\rho_{\text{min}} = -0.59 \text{ e \AA}^{-3}$
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.1201 (2)	0.7351 (3)	0.60899 (13)	0.0310 (5)	
C2	0.0762 (2)	0.6757 (3)	0.66454 (15)	0.0413 (6)	
H1	0.0794	0.5863	0.6690	0.050*	
C3	0.0284 (2)	0.7464 (3)	0.71266 (16)	0.0464 (7)	
H2	-0.0004	0.7041	0.7490	0.056*	
C4	0.0225 (3)	0.8791 (3)	0.70797 (17)	0.0535 (8)	
H3	-0.0088	0.9266	0.7412	0.064*	
C5	0.0635 (3)	0.9394 (3)	0.65357 (18)	0.0510 (8)	
H4	0.0589	1.0288	0.6498	0.061*	
C6	0.1127 (2)	0.8705 (3)	0.60289 (15)	0.0377 (6)	
C7	0.1553 (3)	0.9448 (3)	0.54848 (17)	0.0450 (7)	
H5	0.1532	1.0343	0.5522	0.054*	
C8	0.2543 (9)	0.9774 (6)	0.4478 (4)	0.0442 (17)	0.72 (2)
H6	0.2241	1.0643	0.4428	0.053*	
H7	0.3337	0.9824	0.4701	0.053*	
C9	0.2369 (9)	0.9143 (5)	0.3736 (4)	0.0434 (19)	0.72 (2)
H9	0.1617	0.9311	0.3452	0.052*	
H8	0.2901	0.9473	0.3460	0.052*	
C10	0.2881 (2)	0.7069 (3)	0.33908 (15)	0.0438 (7)	
H10	0.3171	0.7489	0.3028	0.053*	
C11	0.2860 (2)	0.5681 (3)	0.33729 (14)	0.0344 (5)	
C12	0.3126 (3)	0.5076 (3)	0.27460 (16)	0.0462 (7)	
H11	0.3385	0.5580	0.2401	0.055*	
C13	0.3018 (3)	0.3784 (3)	0.26293 (16)	0.0521 (8)	
H12	0.3207	0.3408	0.2214	0.063*	
C14	0.2622 (3)	0.3039 (3)	0.31397 (17)	0.0500 (7)	
H13	0.2518	0.2158	0.3058	0.060*	
C15	0.2379 (2)	0.3589 (3)	0.37687 (16)	0.0426 (6)	
H14	0.2125	0.3068	0.4109	0.051*	
C16	0.2507 (2)	0.4903 (2)	0.39041 (13)	0.0310 (5)	
C17	0.4417 (3)	0.7572 (3)	0.61542 (19)	0.0522 (8)	
H15	0.3802	0.7787	0.6380	0.078*	
H16	0.4551	0.8272	0.5843	0.078*	

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H17	0.5077	0.7424	0.6535	0.078*	
Cu2	0.20183 (3)	0.71765 (3)	0.471852 (16)	0.03015 (7)	
Eu1	0.279281 (10)	0.471486 (11)	0.579103 (6)	0.02628 (4)	
N1	0.1952 (2)	0.8978 (2)	0.49601 (13)	0.0397 (5)	
N2	0.2534 (2)	0.7769 (2)	0.38641 (13)	0.0413 (5)	
N3	0.40354 (19)	0.4886 (2)	0.73120 (12)	0.0404 (5)	
N4	0.08119 (18)	0.3280 (2)	0.59421 (13)	0.0378 (5)	
N5	0.4077 (2)	0.2526 (2)	0.54166 (14)	0.0434 (6)	
O1	0.16860 (14)	0.66089 (16)	0.56505 (9)	0.0309 (4)	
O2	0.22848 (16)	0.53808 (16)	0.45385 (10)	0.0343 (4)	
O3	0.41493 (16)	0.64166 (19)	0.57093 (12)	0.0463 (5)	
H18	0.4580	0.6326	0.5407	0.056*	
O4	0.32467 (16)	0.5670 (2)	0.70399 (10)	0.0430 (5)	
O5	0.4574 (2)	0.5002 (3)	0.79437 (11)	0.0645 (7)	
O6	0.42138 (17)	0.3997 (2)	0.68870 (11)	0.0470 (5)	
O7	0.15586 (16)	0.3634 (2)	0.64981 (10)	0.0414 (4)	
O8	0.00002 (18)	0.2658 (2)	0.60258 (14)	0.0623 (7)	
O9	0.09572 (17)	0.3610 (2)	0.53148 (11)	0.0503 (5)	
O10	0.31744 (18)	0.23862 (19)	0.56357 (13)	0.0491 (5)	
O11	0.4658 (2)	0.1628 (2)	0.53211 (17)	0.0735 (8)	
O12	0.43392 (16)	0.36900 (18)	0.52960 (11)	0.0417 (4)	
C8'	0.202 (2)	0.9864 (16)	0.4356 (11)	0.045 (4)	0.28 (2)
C9'	0.293 (2)	0.9273 (15)	0.4025 (15)	0.054 (6)	0.28 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0286 (11)	0.0361 (14)	0.0289 (12)	0.0057 (10)	0.0078 (10)	-0.0022 (10)
C2	0.0475 (15)	0.0414 (15)	0.0398 (14)	0.0083 (13)	0.0203 (12)	0.0055 (12)
C3	0.0469 (16)	0.059 (2)	0.0399 (15)	0.0091 (14)	0.0239 (13)	0.0027 (14)
C4	0.0624 (19)	0.059 (2)	0.0455 (16)	0.0185 (16)	0.0265 (15)	-0.0091 (15)
C5	0.067 (2)	0.0382 (16)	0.0532 (18)	0.0131 (15)	0.0241 (16)	-0.0060 (14)
C6	0.0430 (14)	0.0349 (14)	0.0372 (14)	0.0042 (12)	0.0130 (12)	-0.0036 (11)
C7	0.0645 (19)	0.0242 (13)	0.0484 (16)	-0.0005 (12)	0.0167 (15)	-0.0026 (12)
C8	0.050 (4)	0.029 (2)	0.060 (3)	-0.008 (3)	0.028 (3)	0.002 (2)
C9	0.066 (5)	0.031 (2)	0.041 (3)	0.002 (3)	0.026 (3)	0.008 (2)
C10	0.0550 (17)	0.0459 (16)	0.0376 (14)	0.0043 (14)	0.0254 (13)	0.0102 (13)
C11	0.0353 (13)	0.0424 (15)	0.0273 (12)	0.0026 (11)	0.0109 (10)	0.0014 (11)
C12	0.0509 (16)	0.060 (2)	0.0321 (14)	0.0063 (14)	0.0184 (12)	0.0022 (13)
C13	0.0574 (18)	0.067 (2)	0.0340 (14)	0.0060 (16)	0.0144 (14)	-0.0165 (15)
C14	0.0586 (18)	0.0465 (17)	0.0452 (16)	-0.0046 (14)	0.0116 (14)	-0.0187 (14)
C15	0.0552 (17)	0.0373 (15)	0.0382 (14)	-0.0068 (13)	0.0162 (13)	-0.0059 (12)
C16	0.0326 (12)	0.0361 (14)	0.0240 (11)	0.0000 (10)	0.0056 (10)	-0.0041 (10)
C17	0.0521 (17)	0.0452 (17)	0.0592 (19)	-0.0135 (14)	0.0119 (15)	-0.0148 (15)
Cu2	0.03982 (16)	0.02575 (15)	0.02774 (14)	-0.00171 (13)	0.01360 (12)	0.00176 (12)
Eu1	0.03128 (7)	0.02506 (7)	0.02520 (6)	-0.00126 (5)	0.01204 (5)	0.00007 (5)
N1	0.0573 (14)	0.0278 (11)	0.0368 (12)	-0.0056 (11)	0.0164 (11)	0.0005 (10)
N2	0.0560 (14)	0.0316 (12)	0.0436 (13)	0.0033 (11)	0.0272 (11)	0.0079 (10)

N3	0.0397 (12)	0.0537 (15)	0.0298 (11)	0.0027 (11)	0.0117 (10)	0.0038 (11)
N4	0.0332 (11)	0.0355 (12)	0.0457 (13)	-0.0022 (9)	0.0106 (10)	0.0097 (10)
N5	0.0463 (13)	0.0380 (13)	0.0491 (14)	0.0035 (11)	0.0173 (11)	-0.0083 (11)
O1	0.0397 (9)	0.0275 (9)	0.0291 (8)	0.0044 (7)	0.0157 (7)	0.0013 (7)
O2	0.0518 (11)	0.0280 (9)	0.0265 (8)	-0.0031 (8)	0.0162 (8)	-0.0011 (7)
O3	0.0473 (11)	0.0414 (11)	0.0589 (12)	-0.0149 (9)	0.0310 (10)	-0.0169 (10)
O4	0.0463 (11)	0.0488 (12)	0.0336 (9)	0.0112 (9)	0.0082 (8)	-0.0057 (9)
O5	0.0611 (14)	0.101 (2)	0.0282 (10)	0.0171 (13)	0.0023 (10)	-0.0018 (12)
O6	0.0515 (12)	0.0453 (12)	0.0432 (11)	0.0133 (10)	0.0081 (9)	-0.0024 (10)
O7	0.0412 (10)	0.0502 (12)	0.0345 (10)	-0.0073 (9)	0.0115 (8)	0.0065 (9)
O8	0.0444 (12)	0.0700 (16)	0.0719 (15)	-0.0220 (11)	0.0114 (11)	0.0244 (13)
O9	0.0476 (11)	0.0671 (15)	0.0355 (10)	-0.0177 (10)	0.0075 (9)	0.0069 (10)
O10	0.0553 (12)	0.0333 (10)	0.0674 (14)	-0.0063 (9)	0.0328 (11)	-0.0066 (10)
O11	0.0754 (16)	0.0431 (13)	0.113 (2)	0.0172 (12)	0.0450 (16)	-0.0089 (14)
O12	0.0458 (10)	0.0358 (10)	0.0498 (11)	-0.0023 (9)	0.0244 (9)	-0.0041 (9)
C8'	0.043 (10)	0.040 (7)	0.059 (9)	-0.004 (7)	0.026 (8)	0.009 (6)
C9'	0.068 (12)	0.034 (6)	0.068 (13)	-0.001 (7)	0.030 (11)	0.010 (7)

Geometric parameters (Å, °)

C1—O1	1.343 (3)	C15—C16	1.387 (4)
C1—C2	1.396 (4)	C15—H14	0.9300
C1—C6	1.408 (4)	C16—O2	1.349 (3)
C2—C3	1.373 (4)	C17—O3	1.448 (3)
C2—H1	0.9300	C17—H15	0.9600
C3—C4	1.379 (5)	C17—H16	0.9600
C3—H2	0.9300	C17—H17	0.9600
C4—C5	1.364 (5)	Cu2—N2	1.918 (2)
C4—H3	0.9300	Cu2—N1	1.925 (2)
C5—C6	1.409 (4)	Cu2—O2	1.9301 (18)
C5—H4	0.9300	Cu2—O1	1.9382 (17)
C6—C7	1.447 (4)	Cu2—O8	2.557 (19)
C7—N1	1.270 (4)	Eu1—O2	2.3589 (18)
C7—H5	0.9300	Eu1—O1	2.3662 (17)
C8—C9	1.488 (8)	Eu1—O3	2.4474 (19)
C8—N1	1.505 (7)	Eu1—O4	2.455 (2)
C8—H6	0.9700	Eu1—O7	2.4643 (19)
C8—H7	0.9700	Eu1—O6	2.476 (2)
C9—N2	1.450 (5)	Eu1—O10	2.486 (2)
C9—H9	0.9700	Eu1—O9	2.503 (2)
C9—H8	0.9700	Eu1—O12	2.5050 (19)
C10—N2	1.275 (4)	N3—O5	1.213 (3)
C10—C11	1.439 (4)	N3—O6	1.258 (3)
C10—H10	0.9300	N3—O4	1.278 (3)
C11—C16	1.405 (4)	N4—O8	1.221 (3)
C11—C12	1.412 (4)	N4—O9	1.253 (3)
C12—C13	1.357 (5)	N4—O7	1.270 (3)
C12—H11	0.9300	N5—O11	1.206 (3)
C13—C14	1.382 (5)	N5—O10	1.262 (3)

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C13—H12	0.9300	N5—O12	1.280 (3)
C14—C15	1.380 (4)	O3—H18	0.8500
C14—H13	0.9300	C8'—C9'	1.51 (3)
O1—C1—C2	118.6 (2)	O2—Eu1—O4	139.18 (7)
O1—C1—C6	123.4 (2)	O1—Eu1—O4	77.08 (6)
C2—C1—C6	118.0 (2)	O3—Eu1—O4	75.39 (7)
C3—C2—C1	121.4 (3)	O2—Eu1—O7	125.98 (6)
C3—C2—H1	119.3	O1—Eu1—O7	91.96 (7)
C1—C2—H1	119.3	O3—Eu1—O7	149.33 (7)
C2—C3—C4	121.0 (3)	O4—Eu1—O7	74.26 (7)
C2—C3—H2	119.5	O2—Eu1—O6	151.09 (7)
C4—C3—H2	119.5	O1—Eu1—O6	128.50 (6)
C5—C4—C3	118.7 (3)	O3—Eu1—O6	84.33 (8)
C5—C4—H3	120.6	O4—Eu1—O6	51.72 (7)
C3—C4—H3	120.6	O7—Eu1—O6	80.47 (7)
C4—C5—C6	122.1 (3)	O2—Eu1—O10	100.83 (7)
C4—C5—H4	119.0	O1—Eu1—O10	155.46 (7)
C6—C5—H4	119.0	O3—Eu1—O10	123.09 (7)
C1—C6—C5	118.8 (3)	O4—Eu1—O10	119.28 (7)
C1—C6—C7	124.0 (2)	O7—Eu1—O10	76.76 (7)
C5—C6—C7	117.2 (3)	O6—Eu1—O10	71.70 (7)
N1—C7—C6	125.2 (2)	O2—Eu1—O9	76.36 (6)
N1—C7—H5	117.4	O1—Eu1—O9	83.86 (7)
C6—C7—H5	117.4	O3—Eu1—O9	151.18 (7)
C9—C8—N1	108.0 (5)	O4—Eu1—O9	121.14 (7)
C9—C8—H6	110.1	O7—Eu1—O9	51.14 (6)
N1—C8—H6	110.1	O6—Eu1—O9	124.49 (7)
C9—C8—H7	110.1	O10—Eu1—O9	72.05 (7)
N1—C8—H7	110.1	O2—Eu1—O12	80.12 (7)
H6—C8—H7	108.4	O1—Eu1—O12	140.39 (6)
N2—C9—C8	107.2 (5)	O3—Eu1—O12	73.07 (7)
N2—C9—H9	110.3	O4—Eu1—O12	118.43 (7)
C8—C9—H9	110.3	O7—Eu1—O12	126.55 (7)
N2—C9—H8	110.3	O6—Eu1—O12	73.59 (7)
C8—C9—H8	110.3	O10—Eu1—O12	51.07 (6)
H9—C9—H8	108.5	O9—Eu1—O12	111.60 (7)
N2—C10—C11	125.3 (2)	C7—N1—C8	123.4 (3)
N2—C10—H10	117.4	C7—N1—Cu2	126.17 (19)
C11—C10—H10	117.4	C8—N1—Cu2	110.2 (3)
C16—C11—C12	118.3 (3)	C10—N2—C9	120.2 (3)
C16—C11—C10	124.3 (2)	C10—N2—Cu2	126.5 (2)
C12—C11—C10	117.2 (2)	C9—N2—Cu2	112.9 (2)
C13—C12—C11	122.4 (3)	O5—N3—O6	122.6 (2)
C13—C12—H11	118.8	O5—N3—O4	121.4 (2)
C11—C12—H11	118.8	O6—N3—O4	116.1 (2)
C12—C13—C14	118.7 (3)	O8—N4—O9	122.7 (2)
C12—C13—H12	120.7	O8—N4—O7	120.9 (2)
C14—C13—H12	120.7	O9—N4—O7	116.4 (2)
C15—C14—C13	120.7 (3)	O11—N5—O10	122.8 (3)

C15—C14—H13	119.7	O11—N5—O12	121.6 (3)
C13—C14—H13	119.7	O10—N5—O12	115.6 (2)
C14—C15—C16	121.4 (3)	C1—O1—Cu2	124.30 (15)
C14—C15—H14	119.3	C1—O1—Eu1	136.48 (15)
C16—C15—H14	119.3	Cu2—O1—Eu1	97.16 (7)
O2—C16—C15	118.7 (2)	C16—O2—Cu2	125.12 (16)
O2—C16—C11	122.8 (2)	C16—O2—Eu1	132.82 (16)
C15—C16—C11	118.5 (2)	Cu2—O2—Eu1	97.62 (7)
N2—Cu2—N1	85.22 (10)	C17—O3—Eu1	129.40 (17)
N2—Cu2—O2	94.04 (9)	C17—O3—H18	111.5
N1—Cu2—O2	172.68 (10)	Eu1—O3—H18	118.9
N2—Cu2—O1	172.90 (9)	N3—O4—Eu1	96.31 (15)
N1—Cu2—O1	93.58 (8)	N3—O6—Eu1	95.84 (15)
O2—Cu2—O1	86.27 (7)	N4—O7—Eu1	96.93 (14)
O2—Eu1—O1	68.07 (6)	N4—O9—Eu1	95.52 (14)
O2—Eu1—O3	76.59 (7)	N5—O10—Eu1	97.13 (15)
O1—Eu1—O3	76.97 (7)	N5—O12—Eu1	95.71 (14)
O1—C1—C2—C3	178.1 (3)	O10—Eu1—O2—C16	-23.4 (2)
C6—C1—C2—C3	-0.9 (4)	O9—Eu1—O2—C16	-91.8 (2)
C1—C2—C3—C4	-0.3 (5)	O12—Eu1—O2—C16	23.5 (2)
C2—C3—C4—C5	1.1 (5)	O1—Eu1—O2—Cu2	23.20 (7)
C3—C4—C5—C6	-0.8 (5)	O3—Eu1—O2—Cu2	-57.94 (8)
O1—C1—C6—C5	-177.8 (3)	O4—Eu1—O2—Cu2	-10.21 (13)
C2—C1—C6—C5	1.1 (4)	O7—Eu1—O2—Cu2	98.92 (9)
O1—C1—C6—C7	0.6 (4)	O6—Eu1—O2—Cu2	-108.02 (13)
C2—C1—C6—C7	179.5 (3)	O10—Eu1—O2—Cu2	-179.67 (7)
C4—C5—C6—C1	-0.3 (5)	O9—Eu1—O2—Cu2	112.00 (9)
C4—C5—C6—C7	-178.8 (3)	O12—Eu1—O2—Cu2	-132.73 (8)
C1—C6—C7—N1	6.4 (5)	O2—Eu1—O3—C17	125.7 (2)
C5—C6—C7—N1	-175.1 (3)	O1—Eu1—O3—C17	55.5 (2)
N1—C8—C9—N2	-43.7 (12)	O4—Eu1—O3—C17	-24.3 (2)
N2—C10—C11—C16	-3.7 (5)	O7—Eu1—O3—C17	-15.8 (3)
N2—C10—C11—C12	171.0 (3)	O6—Eu1—O3—C17	-76.2 (2)
C16—C11—C12—C13	2.2 (4)	O10—Eu1—O3—C17	-140.0 (2)
C10—C11—C12—C13	-172.8 (3)	O9—Eu1—O3—C17	105.1 (3)
C11—C12—C13—C14	0.7 (5)	O12—Eu1—O3—C17	-150.8 (3)
C12—C13—C14—C15	-2.3 (5)	O5—N3—O4—Eu1	177.3 (2)
C13—C14—C15—C16	1.0 (5)	O6—N3—O4—Eu1	-2.7 (2)
C14—C15—C16—O2	-178.3 (3)	O2—Eu1—O4—N3	-140.82 (15)
C14—C15—C16—C11	1.9 (4)	O1—Eu1—O4—N3	-172.43 (16)
C12—C11—C16—O2	176.8 (2)	O3—Eu1—O4—N3	-92.76 (16)
C10—C11—C16—O2	-8.7 (4)	O7—Eu1—O4—N3	91.77 (16)
C12—C11—C16—C15	-3.4 (4)	O6—Eu1—O4—N3	1.58 (14)
C10—C11—C16—C15	171.2 (3)	O10—Eu1—O4—N3	27.29 (18)
C6—C7—N1—C8	-170.4 (5)	O9—Eu1—O4—N3	113.04 (16)
C6—C7—N1—Cu2	3.7 (5)	O12—Eu1—O4—N3	-31.66 (17)
C9—C8—N1—C7	-151.1 (7)	O5—N3—O6—Eu1	-177.3 (2)
C9—C8—N1—Cu2	34.0 (10)	O4—N3—O6—Eu1	2.7 (2)
N2—Cu2—N1—C7	173.2 (3)	O2—Eu1—O6—N3	122.81 (17)

supplementary materials

O1—Cu2—N1—C7	-13.8 (3)	O1—Eu1—O6—N3	5.87 (19)
N2—Cu2—N1—C8	-12.0 (4)	O3—Eu1—O6—N3	74.25 (16)
O1—Cu2—N1—C8	161.0 (4)	O4—Eu1—O6—N3	-1.60 (14)
C11—C10—N2—C9	-166.5 (5)	O7—Eu1—O6—N3	-79.02 (16)
C11—C10—N2—Cu2	5.7 (5)	O10—Eu1—O6—N3	-158.11 (17)
C8—C9—N2—C10	-151.6 (7)	O9—Eu1—O6—N3	-106.50 (16)
C8—C9—N2—Cu2	35.1 (10)	O12—Eu1—O6—N3	148.23 (17)
N1—Cu2—N2—C10	174.0 (3)	O8—N4—O7—Eu1	178.6 (2)
O2—Cu2—N2—C10	1.3 (3)	O9—N4—O7—Eu1	-1.6 (2)
N1—Cu2—N2—C9	-13.2 (5)	O2—Eu1—O7—N4	17.35 (18)
O2—Cu2—N2—C9	174.1 (5)	O1—Eu1—O7—N4	81.45 (15)
C2—C1—O1—Cu2	164.73 (18)	O3—Eu1—O7—N4	148.83 (15)
C6—C1—O1—Cu2	-16.4 (3)	O4—Eu1—O7—N4	157.44 (16)
C2—C1—O1—Eu1	-35.6 (3)	O6—Eu1—O7—N4	-149.81 (16)
C6—C1—O1—Eu1	143.3 (2)	O10—Eu1—O7—N4	-76.52 (16)
N1—Cu2—O1—C1	19.80 (19)	O9—Eu1—O7—N4	0.94 (14)
O2—Cu2—O1—C1	-167.54 (19)	O12—Eu1—O7—N4	-88.56 (16)
N1—Cu2—O1—Eu1	-146.22 (9)	O8—N4—O9—Eu1	-178.7 (2)
O2—Cu2—O1—Eu1	26.44 (7)	O7—N4—O9—Eu1	1.6 (2)
O2—Eu1—O1—C1	173.8 (2)	O2—Eu1—O9—N4	-167.35 (17)
O3—Eu1—O1—C1	-105.6 (2)	O1—Eu1—O9—N4	-98.47 (16)
O4—Eu1—O1—C1	-27.9 (2)	O3—Eu1—O9—N4	-146.72 (15)
O7—Eu1—O1—C1	45.5 (2)	O4—Eu1—O9—N4	-27.60 (19)
O6—Eu1—O1—C1	-33.9 (2)	O7—Eu1—O9—N4	-0.95 (15)
O10—Eu1—O1—C1	107.0 (2)	O6—Eu1—O9—N4	34.82 (19)
O9—Eu1—O1—C1	96.0 (2)	O10—Eu1—O9—N4	86.29 (17)
O12—Eu1—O1—C1	-147.2 (2)	O12—Eu1—O9—N4	119.27 (16)
O2—Eu1—O1—Cu2	-23.08 (6)	O11—N5—O10—Eu1	173.6 (3)
O3—Eu1—O1—Cu2	57.52 (7)	O12—N5—O10—Eu1	-6.8 (2)
O4—Eu1—O1—Cu2	135.25 (8)	O2—Eu1—O10—N5	71.73 (17)
O7—Eu1—O1—Cu2	-151.39 (7)	O1—Eu1—O10—N5	131.96 (17)
O6—Eu1—O1—Cu2	129.24 (8)	O3—Eu1—O10—N5	-9.2 (2)
O10—Eu1—O1—Cu2	-89.87 (16)	O4—Eu1—O10—N5	-100.39 (17)
O9—Eu1—O1—Cu2	-100.81 (8)	O7—Eu1—O10—N5	-163.56 (18)
O12—Eu1—O1—Cu2	15.99 (13)	O6—Eu1—O10—N5	-79.37 (17)
C15—C16—O2—Cu2	-162.6 (2)	O9—Eu1—O10—N5	143.41 (18)
C11—C16—O2—Cu2	17.2 (3)	O12—Eu1—O10—N5	4.01 (15)
C15—C16—O2—Eu1	46.6 (3)	O11—N5—O12—Eu1	-173.7 (3)
C11—C16—O2—Eu1	-133.5 (2)	O10—N5—O12—Eu1	6.7 (2)
N2—Cu2—O2—C16	-12.5 (2)	O2—Eu1—O12—N5	-116.63 (16)
O1—Cu2—O2—C16	174.6 (2)	O1—Eu1—O12—N5	-153.03 (14)
N2—Cu2—O2—Eu1	146.33 (9)	O3—Eu1—O12—N5	164.50 (17)
O1—Cu2—O2—Eu1	-26.56 (7)	O4—Eu1—O12—N5	102.18 (16)
O1—Eu1—O2—C16	179.4 (2)	O7—Eu1—O12—N5	11.19 (18)
O3—Eu1—O2—C16	98.3 (2)	O6—Eu1—O12—N5	75.53 (16)
O4—Eu1—O2—C16	146.0 (2)	O10—Eu1—O12—N5	-3.94 (15)
O7—Eu1—O2—C16	-104.8 (2)	O9—Eu1—O12—N5	-45.68 (17)
O6—Eu1—O2—C16	48.2 (3)		

Hydrogen-bond geometry (Å, °)

$D\text{---H}\cdots A$	$D\text{---H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{---H}\cdots A$
O3—H18 \cdots O12 ⁱ	0.85	2.04	2.886 (3)	174

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

supplementary materials

Fig. 1

