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catena-Poly[[[pentaaquaeuropium(III)]-μ-5-sulfonatoisophthalato-$\kappa^4O^1,O^{1'}:O^3,O^{3'}$] 4,4′-bipyridine *N*,*N*′-dioxide hemisolvate trihydrate]

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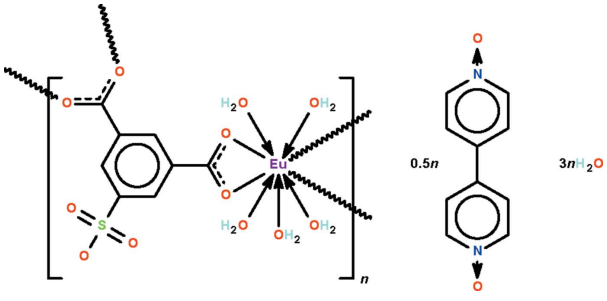
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.032; wR factor = 0.091; data-to-parameter ratio = 16.1.

In the crystal structure of the title compound, $\{[Eu(C_8H_3O_7S)(H_2O)_5]\cdot 0.5C_{10}H_8N_2O_2\cdot 3H_2O\}_n$, the Eu^{III} coordination polymer displays a ribbon motif as the 5-sulfoisopthalate anion uses one of carboxyl $-CO_2$ units to chelate to a Eu atom and the other to bind to other two Eu atoms; the sulfonyl $-SO_3$ unit is not involved in coordination. Adjacent ribbons are linked by O—H···O hydrogen bonds, generating a three-dimensional network. The 4,4′-bipyridine-*N*,*N*′-dioxide molecule lies on an inversion centre and is hydrogen-bonded to the complex network. The coordination geometry of the Eu atom is a monocapped square antiprism.

Related literature

For a related structure, see: Hu *et al.* (2005).



Experimental

Crystal data

$[Eu(C_8H_3O_7S)(H_2O)_5]\cdot 0.5C_{10}H_8N_2O_2\cdot 3H_2O$
M_r = 633.34
Triclinic, $P\overline{1}$
a = 10.7800 (4) Å
b = 10.8978 (3) Å
c = 11.4048 (3) Å
α = 89.383 (2)°
β = 62.989 (1)°
γ = 62.678 (6)°
V = 1026.90 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.24 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.631, T_{max} = 1.000
10108 measured reflections
4658 independent reflections
4509 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.091
S = 1.20
4658 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 3.40 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O8	0.84	1.87	2.673 (4)	159
O1w—H12···O6w	0.84	1.91	2.710 (4)	160
O2w—H22···O1^{i}	0.84	2.11	2.804 (4)	140
O2w—H21···O3w^{i}	0.84	2.46	3.148 (5)	140
O3w—H31···O7w	0.84	1.91	2.742 (4)	175
O3w—H32···O8w	0.84	1.87	2.704 (4)	172
O4w—H41···O8^{ii}	0.83	1.82	2.648 (4)	171
O4w—H42···O5^{iii}	0.83	2.02	2.840 (4)	166
O5w—H51···O7w	0.83	2.30	3.026 (5)	146
O6w—H62···O6^{iv}	0.85	2.18	2.955 (5)	151
O6w—H61···O6^{v}	0.85	2.18	2.807 (5)	130
O7w—H71···O1^{i}	0.84	2.49	3.191 (4)	142
O7w—H72···O7^{vi}	0.84	2.03	2.860 (5)	169
O8w—H81···O2^{vii}	0.85	2.17	2.867 (4)	140
O8w—H82···O5^{viii}	0.85	2.07	2.879 (5)	159

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $-x, -y+2, -z+1$; (iii) $x-1, y, z$; (iv) $-x+1, -y+2, -z+1$; (v) $x-1, y+1, z$; (vi) $x, y, z-1$; (vii) $-x+1, -y+1, -z$; (viii) $-x+2, -y+1, -z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Guangzhou University of Chinese Medicine and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5055).

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supplementary materials

Acta Cryst. (2010). E**66**, m1433 [**doi:10.1107/S1600536810041838**]

catena-Poly[[[pentaaquaeuropium(III)]-μ-5-sulfonatoisophthalato-$\kappa^4O^1,O^{1'}:O^3,O^{3'}$] 4,4'-bipyridine *N*,*N*'-dioxide hemisolvate trihydrate]

A.-Z. Wu and S. W. Ng

Comment

In the crystal structure of pentaqua(5-sulfoisophthalato)europium monohydrate sesqui-4,4'-bipyridine, the 5-sulfoisophthalate trianion *O*,*O*'-chelates to two metal atoms to furnish a polymeric chain structure. The chains are linked by hydrogen bonds into a three-dimensional network, and the *N*-heterocycles occupy the cavities of the network. The geometry of the metal atom is a monocapped square-antiprism (Hu *et al.*, 2005). A similar hydrothermal synthesis with 4,4'-bipyridine *N*-oxide in place of 4,4'-bipyridine affords the corresponding co-crystal, but the co-crystal is a trihydrated1:0.5 co-crystal. In $Eu(H_2O)_5(C_8H_3O_7S)\cdot 3H_2O\cdot 0.5C_{10}H_8N_2O_2$ (Scheme I), the 5-sulfoisopthalate group uses one of carboxyl $–CO_2$ units to chelate to a Eu(III) atom and uses the other to bind to two other metal atoms; the sulfonyl $–SO_3$ unit is not involved in coordination (Fig. 1). The geometry of the europium atom is a monocapped square-antiprism (Fig. 2). Adjacent ribbons (Fig. 3) are linked by O–H···O hydrogen bonds to generate a three-dimensional network (Table 3). The 4,4'-bipyridine *N*-oxide molecule, which lies on a center-of-inversion, is hydrogen-bonded to the network.

Experimental

Europium nitrate hexahydrate (0.22 g, 0.5 mmol), monosodium 5-sulfoisophthalate (0.16 g, 0.5 mmol) and 4,4'-bipyridine-N,N'-dioxide (0.095 g, 0.5 mmol) were placed in a 25-ml Teflon-lined, stainless-steel Parr bomb along with water (15 ml). The bomb was heated to 433 K for 72 h. It was then cooled down to room temperature at a rate of 5 K an hour. Colorless crystals were collected and washed with water (0.195 g, yield 55% based on Eu). The product is stable in air and and is insoluble in water and common organic solvents. CH&N elemental analysis. Calc. for $C_{18}H_{25}N_2EuO_{16}S$ (709.42): C 34.45, H 3.55, N 3.97%. Found: C 34.24, H 3.50, N 4.08%.

Refinement

Carbon-bound hydrogen atoms were placed in calculated positions (C–H 0.93 Å, U_{iso}(H) 1.2 times U_{eq}(C), and were included in the refinement in the riding model approximation. The water H-atoms were placed placed in calculated positions (O–H 0.84 Å and H···H 1.37 Å) on the basis of hydrogen bonding; their temperature factors were tied by a factor of 1.5.

The final difference Fourier map had a peak and a hole in the vicinity of Eu1, but was otherwise featureless. Attempts to decrease their magnitudes by lowering the 2-theta limit did not lower these values, and the structure did not exhibit any signs of twinning.

Figures

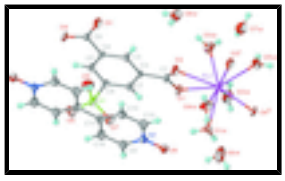

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of a portion of the polymeric structure of $Eu(H_2O)_5(C_8H_3O_7S)\cdot 3H_2O\cdot 0.5C_{10}H_8N_2O_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The 4,4'-bipyridine *N*-oxide molecule lies on a center-of-inversion.

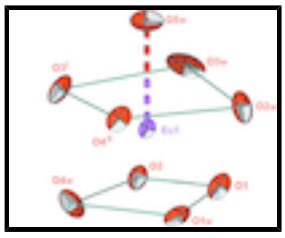

Fig. 2. Nine-coordinate geometry of Eu.

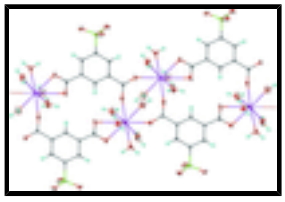

Fig. 3. Ribbon structure.

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Crystal data

$[Eu(C_8H_3O_7S)(H_2O)_5]\cdot 0.5C_{10}H_8N_2O_2\cdot 3H_2O$	$Z = 2$
$M_r = 633.34$	$F(000) = 630$
Triclinic, $P\overline{1}$	$D_x = 2.048$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 10.7800$ (4) Å	Cell parameters from 9807 reflections
$b = 10.8978$ (3) Å	$\theta = 3.5$–$27.5°$
$c = 11.4048$ (3) Å	$\mu = 3.24$ mm^{-1}
$\alpha = 89.383$ (2)°	$T = 293$ K
$\beta = 62.989$ (1)°	Prism, colorless
$\gamma = 62.678$ (6)°	0.25 × 0.20 × 0.15 mm
$V = 1026.90$ (9) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	4658 independent reflections
Radiation source: fine-focus sealed tube	4509 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.033$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 3.5°$
ω scans	$h = -13\rightarrow13$
Absorption correction: multi-scan	$k = -14\rightarrow14$

(*ABSCOR*; Higashi, 1995)
T_{min} = 0.631, T_{max} = 1.000
10108 measured reflections

l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.091
S = 1.20
4658 reflections
289 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.4859P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 3.40 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Eu1	0.222361 (16)	0.944055 (13)	0.073400 (13)	0.01756 (8)
S1	0.84263 (11)	0.67200 (9)	0.32120 (9)	0.02471 (18)
O1	0.4314 (3)	0.8569 (3)	0.1429 (3)	0.0305 (6)
O2	0.3992 (3)	0.6830 (3)	0.0953 (3)	0.0285 (5)
O3	0.8412 (4)	0.1844 (3)	0.0243 (3)	0.0346 (6)
O4	0.9706 (3)	0.1556 (3)	0.1368 (3)	0.0295 (6)
O5	1.0036 (4)	0.6411 (4)	0.2226 (3)	0.0418 (7)
O6	0.8400 (4)	0.6030 (3)	0.4321 (3)	0.0396 (7)
O7	0.7229 (4)	0.8236 (3)	0.3736 (3)	0.0375 (6)
O8	0.1731 (4)	0.9846 (3)	0.4955 (3)	0.0329 (6)
O1W	0.1051 (3)	1.0804 (3)	0.3032 (3)	0.0310 (6)
H11	0.1453	1.0318	0.3474	0.047*
H12	0.0801	1.1650	0.3258	0.047*
O2W	0.3042 (4)	1.1235 (3)	0.0498 (4)	0.0410 (7)
H21	0.3387	1.1230	0.1028	0.061*
H22	0.3771	1.1045	−0.0306	0.061*
O3W	0.4909 (4)	0.8044 (3)	−0.1330 (3)	0.0506 (9)
H31	0.5216	0.8429	−0.1957	0.076*
H32	0.5598	0.7170	−0.1571	0.076*
O4W	0.0462 (4)	0.8763 (3)	0.2470 (3)	0.0410 (7)
H41	−0.0306	0.9237	0.3254	0.061*
H42	0.0447	0.8044	0.2251	0.061*
O5W	0.2265 (4)	1.0292 (4)	−0.1370 (3)	0.0441 (8)
H51	0.3014	1.0388	−0.1953	0.066*
H52	0.1451	1.0708	−0.1456	0.066*
O6W	0.1006 (6)	1.3246 (4)	0.3568 (5)	0.0661 (12)
H61	0.0007	1.3802	0.4141	0.099*

H62	0.1513	1.3186	0.3980	0.099*
O7W	0.5761 (4)	0.9318 (4)	−0.3410 (3)	0.0442 (8)
H71	0.6177	0.9731	−0.3246	0.066*
H72	0.6113	0.9114	−0.4245	0.066*
O8W	0.6904 (4)	0.5181 (3)	−0.2118 (3)	0.0423 (7)
H81	0.6327	0.4968	−0.1455	0.064*
H82	0.7768	0.4929	−0.2110	0.064*
N1	0.2607 (4)	0.8511 (3)	0.4986 (3)	0.0260 (6)
C1	0.4710 (4)	0.7263 (4)	0.1275 (3)	0.0211 (6)
C2	0.6071 (4)	0.6265 (3)	0.1492 (3)	0.0182 (6)
C3	0.6773 (4)	0.4793 (3)	0.1120 (3)	0.0199 (6)
H3	0.6427	0.4402	0.0698	0.024*
C4	0.7996 (4)	0.3904 (3)	0.1383 (3)	0.0185 (6)
C5	0.8531 (4)	0.4479 (3)	0.1990 (3)	0.0216 (6)
H5	0.9366	0.3882	0.2142	0.026*
C6	0.7815 (4)	0.5957 (3)	0.2375 (4)	0.0217 (6)
C7	0.6609 (4)	0.6842 (3)	0.2107 (3)	0.0203 (6)
H7	0.6157	0.7825	0.2338	0.024*
C8	0.8774 (4)	0.2302 (3)	0.0962 (3)	0.0201 (6)
C9	0.3563 (5)	0.8243 (4)	0.5518 (4)	0.0305 (8)
H9	0.3592	0.8988	0.5872	0.037*
C10	0.4495 (5)	0.6877 (4)	0.5543 (4)	0.0320 (8)
H10	0.5150	0.6705	0.5916	0.038*
C11	0.4475 (4)	0.5746 (4)	0.5022 (3)	0.0248 (7)
C12	0.3437 (5)	0.6074 (4)	0.4505 (4)	0.0292 (7)
H12A	0.3361	0.5351	0.4174	0.035*
C13	0.2525 (5)	0.7454 (4)	0.4480 (4)	0.0311 (8)
H13	0.1856	0.7657	0.4116	0.037*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Eu1	0.01783 (11)	0.01261 (11)	0.02442 (12)	−0.00607 (8)	−0.01399 (8)	0.00504 (7)
S1	0.0289 (4)	0.0182 (4)	0.0365 (4)	−0.0127 (3)	−0.0228 (4)	0.0062 (3)
O1	0.0349 (14)	0.0155 (11)	0.0467 (15)	−0.0070 (11)	−0.0306 (13)	0.0079 (11)
O2	0.0316 (14)	0.0250 (12)	0.0428 (14)	−0.0151 (11)	−0.0283 (12)	0.0145 (11)
O3	0.0466 (17)	0.0176 (11)	0.0531 (17)	−0.0123 (12)	−0.0389 (14)	0.0047 (11)
O4	0.0291 (13)	0.0154 (10)	0.0412 (14)	−0.0024 (10)	−0.0248 (12)	0.0052 (10)
O5	0.0353 (16)	0.0459 (17)	0.0472 (17)	−0.0255 (14)	−0.0181 (14)	0.0017 (14)
O6	0.063 (2)	0.0370 (15)	0.0425 (15)	−0.0283 (15)	−0.0416 (15)	0.0158 (13)
O7	0.0460 (17)	0.0197 (12)	0.0515 (17)	−0.0116 (12)	−0.0333 (15)	0.0025 (12)
O8	0.0399 (15)	0.0218 (12)	0.0321 (13)	−0.0094 (12)	−0.0210 (12)	0.0075 (11)
O1W	0.0447 (16)	0.0234 (12)	0.0295 (12)	−0.0136 (11)	−0.0260 (12)	0.0065 (10)
O2W	0.0412 (17)	0.0359 (15)	0.064 (2)	−0.0283 (14)	−0.0311 (16)	0.0240 (15)
O3W	0.0385 (17)	0.0373 (16)	0.0340 (15)	−0.0015 (14)	−0.0059 (13)	0.0146 (13)
O4W	0.0450 (17)	0.0279 (13)	0.0320 (13)	−0.0247 (13)	0.0001 (12)	−0.0031 (11)
O5W	0.0452 (18)	0.0478 (18)	0.0304 (14)	−0.0162 (15)	−0.0202 (13)	0.0166 (14)
O6W	0.085 (3)	0.0321 (17)	0.117 (4)	−0.0247 (19)	−0.082 (3)	0.021 (2)

O7W	0.0430 (18)	0.0456 (18)	0.0454 (18)	−0.0269 (16)	−0.0190 (15)	0.0187 (15)
O8W	0.0333 (15)	0.0390 (16)	0.0533 (18)	−0.0186 (13)	−0.0208 (14)	0.0149 (14)
N1	0.0280 (15)	0.0233 (14)	0.0203 (12)	−0.0103 (12)	−0.0103 (11)	0.0060 (11)
C1	0.0186 (15)	0.0184 (15)	0.0246 (15)	−0.0064 (13)	−0.0130 (13)	0.0089 (13)
C2	0.0204 (14)	0.0155 (14)	0.0199 (13)	−0.0065 (12)	−0.0139 (12)	0.0065 (11)
C3	0.0219 (15)	0.0166 (13)	0.0249 (14)	−0.0090 (12)	−0.0153 (13)	0.0064 (13)
C4	0.0199 (14)	0.0122 (12)	0.0233 (14)	−0.0060 (11)	−0.0131 (12)	0.0038 (11)
C5	0.0213 (15)	0.0163 (14)	0.0290 (15)	−0.0057 (12)	−0.0180 (13)	0.0046 (12)
C6	0.0234 (16)	0.0157 (14)	0.0314 (16)	−0.0099 (13)	−0.0179 (14)	0.0051 (12)
C7	0.0231 (15)	0.0134 (13)	0.0269 (15)	−0.0080 (12)	−0.0157 (13)	0.0054 (12)
C8	0.0193 (14)	0.0132 (13)	0.0257 (15)	−0.0051 (12)	−0.0131 (12)	0.0030 (12)
C9	0.035 (2)	0.0258 (17)	0.0312 (17)	−0.0146 (16)	−0.0185 (16)	0.0045 (15)
C10	0.036 (2)	0.0304 (18)	0.0378 (19)	−0.0156 (16)	−0.0256 (17)	0.0089 (16)
C11	0.0223 (16)	0.0251 (17)	0.0244 (15)	−0.0126 (14)	−0.0095 (13)	0.0096 (13)
C12	0.0340 (19)	0.0270 (17)	0.0312 (17)	−0.0159 (16)	−0.0194 (16)	0.0062 (15)
C13	0.0314 (19)	0.0312 (18)	0.0351 (18)	−0.0151 (16)	−0.0210 (16)	0.0075 (15)

Geometric parameters (Å, °)

Eu1—O1	2.500 (2)	O6W—H61	0.8513
Eu1—O2	2.688 (2)	O6W—H62	0.8503
Eu1—O3^{i}	2.298 (3)	O7W—H71	0.8376
Eu1—O4^{ii}	2.390 (2)	O7W—H72	0.8365
Eu1—O1W	2.455 (2)	O8W—H81	0.8459
Eu1—O2W	2.456 (3)	O8W—H82	0.8457
Eu1—O3W	2.466 (3)	N1—C9	1.343 (5)
Eu1—O4W	2.431 (3)	N1—C13	1.350 (5)
Eu1—O5W	2.552 (3)	C1—C2	1.502 (4)
S1—O5	1.445 (3)	C2—C7	1.391 (4)
S1—O7	1.454 (3)	C2—C3	1.392 (4)
S1—O6	1.460 (3)	C3—C4	1.395 (4)
S1—C6	1.769 (3)	C3—H3	0.9300
O1—C1	1.273 (4)	C4—C5	1.381 (4)
O2—C1	1.246 (4)	C4—C8	1.513 (4)
O3—C8	1.245 (4)	C5—C6	1.396 (4)
O4—C8	1.245 (4)	C5—H5	0.9300
O8—N1	1.333 (4)	C6—C7	1.385 (4)
O1W—H11	0.8386	C7—H7	0.9300
O1W—H12	0.8384	C9—C10	1.371 (5)
O2W—H21	0.8400	C9—H9	0.9300
O2W—H22	0.8380	C10—C11	1.387 (5)
O3W—H31	0.8383	C10—H10	0.9300
O3W—H32	0.8396	C11—C12	1.398 (5)
O4W—H41	0.8345	C11—C11^{iii}	1.479 (7)
O4W—H42	0.8346	C12—C13	1.378 (5)
O5W—H51	0.8333	C12—H12A	0.9300
O5W—H52	0.8349	C13—H13	0.9300
O3^{i}—Eu1—O4^{ii}	90.47 (9)	Eu1—O3W—H32	130.2

O3^{i}—Eu1—O4W	70.06 (11)	H31—O3W—H32	109.5
O4^{ii}—Eu1—O4W	82.34 (10)	Eu1—O4W—H41	129.1
O3^{i}—Eu1—O2W	144.73 (11)	Eu1—O4W—H42	119.2
O4^{ii}—Eu1—O2W	79.72 (10)	H41—O4W—H42	110.4
O4W—Eu1—O2W	140.17 (11)	Eu1—O5W—H51	123.4
O3^{i}—Eu1—O1W	135.51 (11)	Eu1—O5W—H52	124.1
O4^{ii}—Eu1—O1W	70.13 (9)	H51—O5W—H52	110.6
O4W—Eu1—O1W	67.97 (10)	H61—O6W—H62	106.3
O2W—Eu1—O1W	72.54 (11)	H71—O7W—H72	110.2
O3^{i}—Eu1—O3W	82.80 (13)	H81—O8W—H82	107.4
O4^{ii}—Eu1—O3W	137.24 (10)	O8—N1—C9	119.1 (3)
O4W—Eu1—O3W	132.75 (10)	O8—N1—C13	119.7 (3)
O2W—Eu1—O3W	81.93 (12)	C9—N1—C13	121.2 (3)
O1W—Eu1—O3W	138.25 (12)	O2—C1—O1	121.0 (3)
O3^{i}—Eu1—O1	129.26 (8)	O2—C1—C2	121.4 (3)
O4^{ii}—Eu1—O1	137.26 (9)	O1—C1—C2	117.6 (3)
O4W—Eu1—O1	95.95 (11)	C7—C2—C3	119.8 (3)
O2W—Eu1—O1	74.72 (9)	C7—C2—C1	118.7 (3)
O1W—Eu1—O1	69.79 (9)	C3—C2—C1	121.5 (3)
O3W—Eu1—O1	71.94 (11)	C2—C3—C4	119.8 (3)
O3^{i}—Eu1—O5W	72.39 (11)	C2—C3—H3	120.1
O4^{ii}—Eu1—O5W	69.93 (10)	C4—C3—H3	120.1
O4W—Eu1—O5W	132.53 (12)	C5—C4—C3	120.3 (3)
O2W—Eu1—O5W	72.42 (11)	C5—C4—C8	119.9 (3)
O1W—Eu1—O5W	130.36 (10)	C3—C4—C8	119.8 (3)
O3W—Eu1—O5W	67.78 (10)	C4—C5—C6	119.9 (3)
O1—Eu1—O5W	130.58 (11)	C4—C5—H5	120.1
O3^{i}—Eu1—O2	80.16 (8)	C6—C5—H5	120.1
O4^{ii}—Eu1—O2	152.27 (9)	C7—C6—C5	120.0 (3)
O4W—Eu1—O2	69.93 (10)	C7—C6—S1	119.3 (2)
O2W—Eu1—O2	122.10 (9)	C5—C6—S1	120.7 (3)
O1W—Eu1—O2	98.56 (8)	C6—C7—C2	120.2 (3)
O3W—Eu1—O2	67.78 (9)	C6—C7—H7	119.9
O1—Eu1—O2	49.82 (8)	C2—C7—H7	119.9
O5W—Eu1—O2	129.85 (10)	O3—C8—O4	125.6 (3)
O5—S1—O7	113.70 (19)	O3—C8—C4	116.8 (3)
O5—S1—O6	112.2 (2)	O4—C8—C4	117.7 (3)
O7—S1—O6	110.88 (19)	N1—C9—C10	120.3 (4)
O5—S1—C6	107.16 (17)	N1—C9—H9	119.8
O7—S1—C6	106.77 (16)	C10—C9—H9	119.8
O6—S1—C6	105.62 (16)	C9—C10—C11	121.0 (3)
C1—O1—Eu1	98.7 (2)	C9—C10—H10	119.5
C1—O2—Eu1	90.40 (19)	C11—C10—H10	119.5
C8—O3—Eu1^{i}	164.5 (2)	C10—C11—C12	116.8 (3)
C8—O4—Eu1^{iv}	144.6 (2)	C10—C11—C11^{iii}	122.1 (4)

Eu1—O1W—H11	113.1	C12—C11—C11^{iii}	121.0 (4)
Eu1—O1W—H12	126.6	C13—C12—C11	120.9 (3)
H11—O1W—H12	109.5	C13—C12—H12A	119.5
Eu1—O2W—H21	109.7	C11—C12—H12A	119.5
Eu1—O2W—H22	109.1	N1—C13—C12	119.6 (3)
H21—O2W—H22	109.8	N1—C13—H13	120.2
Eu1—O3W—H31	120.1	C12—C13—H13	120.2
O3^{i}—Eu1—O1—C1	−9.5 (3)	C4—C5—C6—C7	−2.2 (5)
O4^{ii}—Eu1—O1—C1	144.7 (2)	C4—C5—C6—S1	177.6 (3)
O4W—Eu1—O1—C1	59.5 (2)	O5—S1—C6—C7	−109.9 (3)
O2W—Eu1—O1—C1	−160.0 (2)	O7—S1—C6—C7	12.3 (3)
O1W—Eu1—O1—C1	123.4 (2)	O6—S1—C6—C7	130.4 (3)
O3W—Eu1—O1—C1	−73.6 (2)	O5—S1—C6—C5	70.4 (3)
O5W—Eu1—O1—C1	−110.2 (2)	O7—S1—C6—C5	−167.5 (3)
O2—Eu1—O1—C1	2.17 (19)	O6—S1—C6—C5	−49.4 (3)
O3^{i}—Eu1—O2—C1	168.6 (2)	C5—C6—C7—C2	2.0 (5)
O4^{ii}—Eu1—O2—C1	−119.5 (2)	S1—C6—C7—C2	−177.8 (3)
O4W—Eu1—O2—C1	−119.1 (2)	C3—C2—C7—C6	−1.3 (5)
O2W—Eu1—O2—C1	18.3 (2)	C1—C2—C7—C6	177.3 (3)
O1W—Eu1—O2—C1	−56.4 (2)	Eu1^{i}—O3—C8—O4	36.9 (12)
O3W—Eu1—O2—C1	82.5 (2)	Eu1^{i}—O3—C8—C4	−142.6 (8)
O1—Eu1—O2—C1	−2.2 (2)	Eu1^{iv}—O4—C8—O3	42.7 (7)
O5W—Eu1—O2—C1	111.6 (2)	Eu1^{iv}—O4—C8—C4	−137.8 (3)
Eu1—O2—C1—O1	3.8 (3)	C5—C4—C8—O3	−169.6 (3)
Eu1—O2—C1—C2	−176.0 (3)	C3—C4—C8—O3	8.6 (5)
Eu1—O1—C1—O2	−4.2 (4)	C5—C4—C8—O4	10.9 (5)
Eu1—O1—C1—C2	175.7 (2)	C3—C4—C8—O4	−170.9 (3)
O2—C1—C2—C7	−167.3 (3)	O8—N1—C9—C10	−179.0 (3)
O1—C1—C2—C7	12.8 (5)	C13—N1—C9—C10	0.8 (6)
O2—C1—C2—C3	11.2 (5)	N1—C9—C10—C11	0.1 (6)
O1—C1—C2—C3	−168.6 (3)	C9—C10—C11—C12	−1.5 (6)
C7—C2—C3—C4	0.8 (5)	C9—C10—C11—C11^{iii}	177.1 (4)
C1—C2—C3—C4	−177.7 (3)	C10—C11—C12—C13	2.2 (6)
C2—C3—C4—C5	−1.0 (5)	C11^{iii}—C11—C12—C13	−176.5 (4)
C2—C3—C4—C8	−179.2 (3)	O8—N1—C13—C12	179.6 (3)
C3—C4—C5—C6	1.7 (5)	C9—N1—C13—C12	−0.1 (6)
C8—C4—C5—C6	179.9 (3)	C11—C12—C13—N1	−1.4 (6)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) *x*−1, *y*+1, *z*; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*+1, *y*−1, *z*.

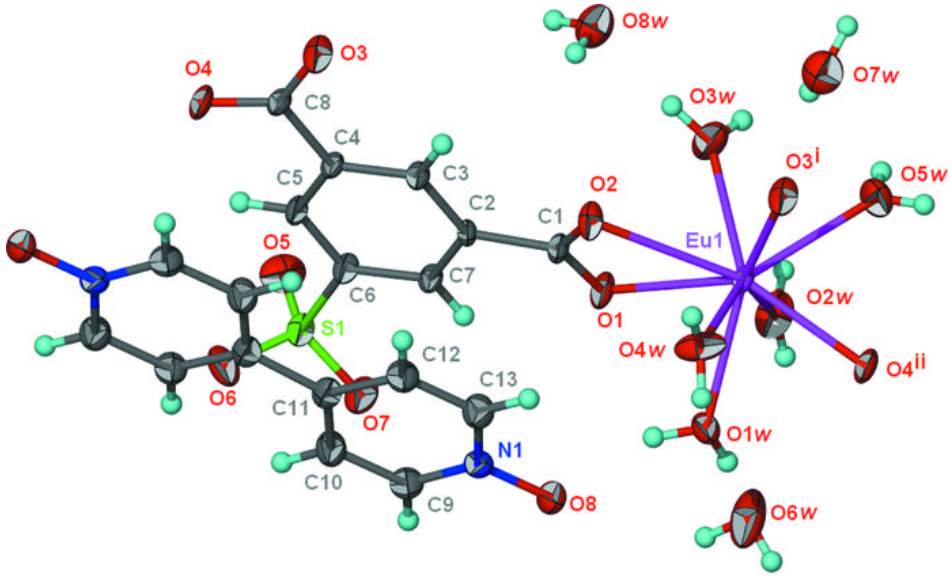
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···O8	0.84	1.87	2.673 (4)	159
O1w—H12···O6w	0.84	1.91	2.710 (4)	160
O2w—H22···O1^{v}	0.84	2.11	2.804 (4)	140
O2w—H21···O3w^{v}	0.84	2.46	3.148 (5)	140

O3w—H31···O7w	0.84	1.91	2.742 (4)	175
O3w—H32···O8w	0.84	1.87	2.704 (4)	172
O4w—H41···O8^{vi}	0.83	1.82	2.648 (4)	171
O4w—H42···O5^{vii}	0.83	2.02	2.840 (4)	166
O5w—H51···O7w	0.83	2.30	3.026 (5)	146
O6w—H62···O6^{viii}	0.85	2.18	2.955 (5)	151
O6w—H61···O6^{ii}	0.85	2.18	2.807 (5)	130
O7w—H71···O1^{v}	0.84	2.49	3.191 (4)	142
O7w—H72···O7^{ix}	0.84	2.03	2.860 (5)	169
O8w—H81···O2^{i}	0.85	2.17	2.867 (4)	140
O8w—H82···O5^{x}	0.85	2.07	2.879 (5)	159

Symmetry codes: (v) −*x*+1, −*y*+2, −*z*; (vi) −*x*, −*y*+2, −*z*+1; (vii) *x*−1, *y*, *z*; (viii) −*x*+1, −*y*+2, −*z*+1; (ii) *x*−1, *y*+1, *z*; (ix) *x*, *y*, *z*−1; (i) −*x*+1, −*y*+1, −*z*; (x) −*x*+2, −*y*+1, −*z*.

Fig. 1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O7w
O3w
O3
O4
C8
C4
C5
C3
C2
C1
O2
O3i
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O5
C7
C6
S1
O1
O2w
O4w
O4ii
C12
C13
O6
C11
O7
N1
O1w
C10
C9
O8
O6w

Fig. 2

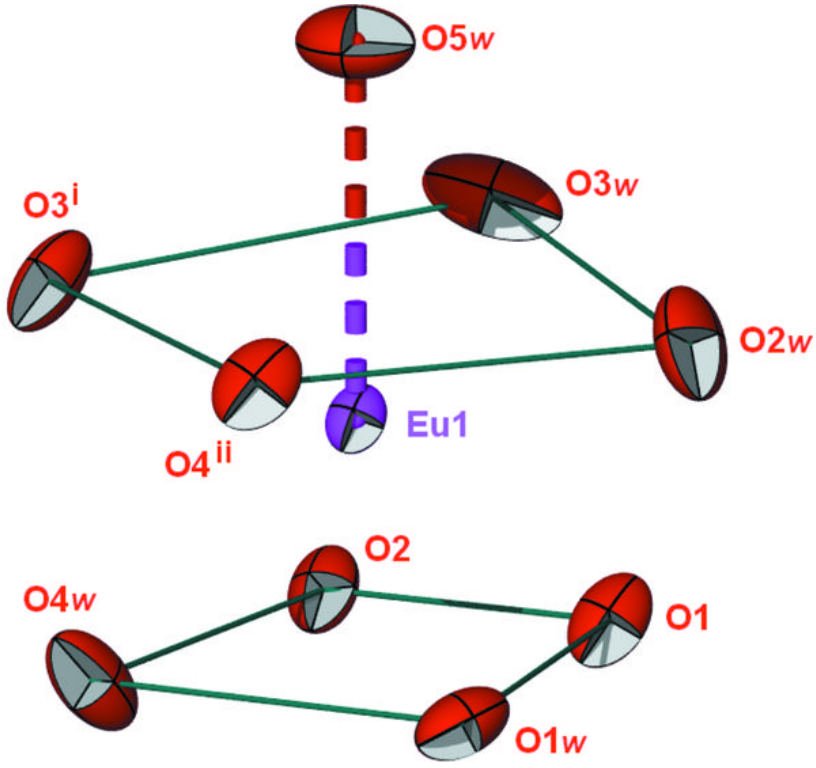

Fig. 3