Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Dimethylaminopyridinium tetrakis-[3,3,3-trifluoro-1-(2-thienylcarbonyl)-prop-1-en-2-olato]europate(III)

Xiu-Cheng Wei,[a] Yu-Kun Bian,[a] Kai-Bei Yu[b] and De-Yan He[a]*

[a]School of Physical Science and Technology, Lanzhou University, Lanzhou 730000, People's Republic of China, and [b]Chengdu Institute of Organic Chemistry, Chinese Academy of Sciences, Chengdu 610041, People's Republic of China
Correspondence e-mail: hedy@lzu.edu.cn

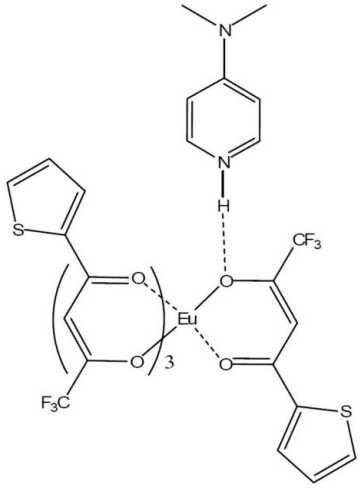
Received 14 August 2007; accepted 17 September 2007

Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.032; wR factor = 0.085; data-to-parameter ratio = 14.0.

The title complex, $(C_7H_{11}N_2)[Eu(C_8H_4F_3O_2S)_4]$ or [DMAP]-[Eu(TTA)$_4$], features a trivalent Eu^{III} cation that is eight-coordinated by eight O atoms derived from four chelating β-diketonate ligands. The range of Eu—O bond distances is 2.3594 (18)–2.4896 (18) Å. The coordination polyhedron is based on a distorted tetragonal antiprism. N—H···O hydrogen bonding connects the cation to the anion. There is twofold flip disorder of two thienyl rings with occupancies in the approximate ratio 2:1; one CF_3 group is equally disordered over two orientations, and another shows extensive disorder, modelled in four different orientations with unequal occupancies.

Related literature

For the corresponding 4-aminopyridinium complex, see Chen *et al.* (2001). For related literature, see: Bauer *et al.* (1964); Sweeting & Rheingold (1987).



Experimental

Crystal data

$(C_7H_{11}N_2)[Eu(C_8H_4F_3O_2S)_4]$
M_r = 1159.83
Orthorhombic, *Pbca*
a = 20.0202 (4) Å
b = 18.9160 (3) Å
c = 23.4108 (4) Å
V = 8865.7 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.71 mm^{-1}
T = 93 (2) K
0.62 × 0.45 × 0.23 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*ABSCOR*; Higashi, 1999)
T_{min} = 0.418, T_{max} = 0.695
82834 measured reflections
10137 independent reflections
9604 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.00
10137 reflections
725 parameters
76 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.29 e Å^{-3}
$\Delta\rho_{min}$ = −1.10 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O6^{i}	0.87 (4)	1.96 (4)	2.814 (3)	168 (4)

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

Data collection: *RAPID-AUTO* (Rigaku, 2006); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1998); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Interdisciplinary Innovation Research Fund for Young Scholars, Lanzhou University, China (grant No. LZU824606), and the Research Award Fund for Outstanding Young Teachers in Higher Education Institutions, China (grant No. 2002363).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2189).

References

Bauer, H., Blanc, J. & Ross, D. L. (1964). *J. Am. Chem. Soc.* **86**, 5125–5131.
Chen, X. F., Duan, C. Y., Zhu, X. H., You, X. Z., Raj, S. S. S., Fun, H. K. & Wu, J. (2001). *Mater. Chem. Phys.* **72**, 11–15.
Higashi, T. (1999). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (2006). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1998). *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sweeting, L. M. & Rheingold, A. L. (1987). *J. Am. Chem. Soc.* **109**, 2652–2658.

  doi:10.1107/S1600536807045667

supplementary materials

Acta Cryst. (2007). E**63**, m2566 [**doi:10.1107/S1600536807045667**]

4-Dimethylaminopyridinium tetrakis[3,3,3-trifluoro-1-(2-thienylcarbonyl)prop-1-en-2-olato]europate(III)

X.-C. Wei, Y.-K. Bian, K.-B. Yu and D.-Y. He

Comment

The structure of the title complex, [DMAP][Eu(TTA)$_4$] (I), Fig. 1, shows the trivalent Eu cation to be 8-coordinated by eight O atoms derived from four chelating β-diketonate ligands. The coordination polyhedron can be best described as a distorted tetragonal antiprism in which the square planes are defined by the O1, O2, O5 & O6 atoms and the atoms O3, O4, O7 & O8. The 4-dimethylaminopyridinium cation forms a N—H···O hydrogen bond to the O6 atom (Table 1). Complex (I) has intensive photoluminescence (PL) at room temperature. The corresponding 4-aminopyridinium complex, [4-aminopyridinium][Eu(TTA)$_4$] has mechanoluminescence (ML) properties (Chen *et al.*, 2001), which was attributed to the disorder in the thienyl rings and CF_3 groups (Sweeting & Rheingold, 1987). However, (I) also has disorder in the thienyl rings and CF_3 groups (see Experimental) but does not exhibit ML.

Experimental

All chemicals were of analytical grade and were used without further purification. Complex (I) was prepared according to method C in Bauer *et al.*, 1964. Pale-yellow products were obtained. Purification by recrystallization was accomplished by room temperature evaporation of a CH_2Cl_2 solution of (I). Single crystal suitable for X-ray analysis were obtained from an EtOH solution of (I); m. pt. 422 K.

Refinement

Two of the four thienyl rings as well as the four CF_3 groups are disordered. The positional disorder of F atoms, F4, F5 and F6, was modelled anisotropically over two positions with site occupancy factors for the primed and unprimed atoms equalling 0.5 (from refinement). The F10, F11 and F12 atoms were modelled over four positions with the site occupancy factors of 0.472, 0.274, 0.099 and 0.156 for atoms (F10, F11, F12), (F10A, F11A, F12A), (F10B, F11B, F12B) and (F10C, F11C, F12C), respectively, as determined from least-squares refinement; of these, the F10, F11, & F12 atoms were refined with anisotropic displacement parameters.

Two of the four thienyl rings were disordered and modelled anisotropically over two orientations with refined occupancy factors of S3:S3'=0.668 (5):0.332 and S4:S4'=0.656 (4):0.344, respectively, obtained from least-squares refinement.

The N1—H atom was located by difference Fourier synthesis and refined without constraint so that N—H = 0.87 Å. The C-bound H atoms were included in the riding model approximation with C—H = 0.95 − 0.98 Å, and with U_{iso}(H) = 1.2U_{eq}(C). The highest residual electron density peak is 0.78Å from the Eu atom, and the deepest hole is 0.62 Å from the S2 atom.

Figures

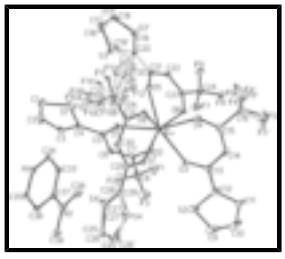


Fig. 1. Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level. H atoms have been omitted for clarity.

4-Dimethylaminopyridinium tetrakis[3,3,3-trifluoro-1-(2-thienylcarbonyl)prop-1-en-2-olato]europate(III)

Crystal data

$(C_7H_{11}N_2)[Eu(C_8H_4F_3O_2S)_4]$	$D_x = 1.738$ Mg m^{-3}
$M_r = 1159.83$	Melting point: 422 K
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 77909 reflections
a = 20.0202 (4) Å	θ = 3.0–27.5º
b = 18.9160 (3) Å	μ = 1.71 mm^{-1}
c = 23.4108 (4) Å	*T* = 93 (2) K
V = 8865.7 (3) Å^3	Block, light yellow
Z = 8	0.62 × 0.45 × 0.23 mm
$F_{000} = 4592$	

Data collection

Rigaku R-AXIS RAPID diffractometer	10137 independent reflections
Radiation source: Rotating Anode	9604 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.048$
T = 93(2) K	$\theta_{max} = 27.5$º
ω scans	$\theta_{min} = 3.0$º
Absorption correction: numerical (ABSCOR; Higashi, 1999)	*h* = −25→21
$T_{min} = 0.418$, $T_{max} = 0.695$	*k* = −24→24
82834 measured reflections	*l* = −30→30

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.085$	$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 19.8P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.002$
10137 reflections	$\Delta\rho_{max} = 1.29$ e Å^{-3}
725 parameters	$\Delta\rho_{min} = -1.10$ e Å^{-3}
76 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00046 (5)

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Eu	0.597426 (6)	0.721987 (6)	0.360975 (5)	0.01510 (6)	
S1	0.60799 (4)	0.57483 (4)	0.17677 (3)	0.03073 (16)	
S2	0.39615 (5)	0.83825 (6)	0.44619 (5)	0.0506 (3)	
F1	0.39394 (12)	0.59604 (15)	0.43360 (8)	0.0594 (7)	
F2	0.34744 (12)	0.57253 (18)	0.35390 (9)	0.0750 (10)	
F3	0.35621 (11)	0.67993 (16)	0.38226 (13)	0.0737 (8)	
F7	0.58142 (9)	0.56142 (11)	0.53956 (8)	0.0405 (5)	
F8	0.65626 (10)	0.63695 (11)	0.56345 (7)	0.0402 (5)	
F9	0.68492 (10)	0.53054 (10)	0.54391 (7)	0.0390 (5)	
O1	0.57171 (10)	0.64663 (11)	0.28185 (8)	0.0270 (4)	
O2	0.49679 (9)	0.66181 (10)	0.38064 (8)	0.0228 (4)	
O3	0.52853 (9)	0.79803 (11)	0.41529 (8)	0.0232 (4)	
O4	0.66577 (9)	0.79900 (10)	0.41878 (8)	0.0220 (4)	
O5	0.68395 (9)	0.63666 (10)	0.35019 (8)	0.0215 (4)	
O6	0.61699 (9)	0.65975 (10)	0.45317 (7)	0.0199 (4)	
O7	0.53810 (9)	0.79814 (11)	0.29734 (8)	0.0243 (4)	
O8	0.67192 (8)	0.76383 (10)	0.29028 (7)	0.0172 (3)	
N1	0.53190 (12)	0.78441 (13)	0.03754 (10)	0.0228 (5)	
N2	0.37594 (13)	0.73141 (14)	0.14289 (10)	0.0276 (5)	
C1	0.5848 (2)	0.5117 (2)	0.12886 (14)	0.0430 (8)	
H1	0.6112	0.4979	0.0970	0.052*	
C2	0.5244 (2)	0.4834 (2)	0.14134 (15)	0.0509 (10)	
H2	0.5039	0.4477	0.1189	0.061*	
C3	0.49566 (16)	0.51149 (15)	0.18959 (11)	0.0280 (6)	

H3	0.4534	0.4972	0.2041	0.034*	
C4	0.53614 (15)	0.56404 (15)	0.21516 (11)	0.0246 (5)	
C5	0.52640 (13)	0.60478 (14)	0.26746 (11)	0.0218 (5)	
C6	0.46612 (14)	0.59541 (16)	0.29869 (11)	0.0273 (6)	
H6	0.4315	0.5675	0.2826	0.033*	
C7	0.45655 (14)	0.62543 (16)	0.35122 (11)	0.0251 (6)	
C8	0.38772 (15)	0.61804 (15)	0.37990 (10)	0.0425 (9)	
C9	0.3482 (2)	0.8823 (3)	0.4915 (2)	0.0627 (13)	
H9	0.3008	0.8809	0.4903	0.075*	
C10	0.3826 (3)	0.9204 (2)	0.5301 (2)	0.0659 (14)	
H10	0.3606	0.9472	0.5587	0.079*	
C11	0.45524 (16)	0.91853 (16)	0.52591 (13)	0.0331 (7)	
H11	0.4870	0.9434	0.5483	0.040*	
C12	0.46776 (16)	0.86778 (15)	0.47749 (13)	0.0300 (6)	
C13	0.53184 (14)	0.84155 (14)	0.45560 (11)	0.0231 (5)	
C14	0.59243 (15)	0.86281 (16)	0.48075 (12)	0.0279 (6)	
H14	0.5916	0.8957	0.5114	0.034*	
C15	0.65323 (14)	0.83693 (15)	0.46199 (11)	0.0243 (5)	
C16	0.71490 (14)	0.85150 (14)	0.49939 (11)	0.0351 (7)	
C21	0.70624 (11)	0.58265 (12)	0.37441 (10)	0.0169 (5)	
C22	0.69243 (12)	0.56499 (14)	0.43225 (11)	0.0198 (5)	
H22	0.7125	0.5239	0.4481	0.024*	
C23	0.65101 (12)	0.60529 (14)	0.46600 (10)	0.0190 (5)	
C24	0.64375 (11)	0.58252 (12)	0.52873 (10)	0.0281 (6)	
C29	0.54665 (12)	0.82280 (13)	0.24797 (10)	0.0205 (5)	
C30	0.60626 (13)	0.81424 (15)	0.21592 (11)	0.0217 (5)	
H30	0.6073	0.8295	0.1773	0.026*	
C31	0.66273 (12)	0.78427 (13)	0.23958 (10)	0.0178 (5)	
C32	0.72446 (12)	0.77568 (12)	0.20115 (9)	0.0268 (6)	
C33	0.49300 (14)	0.72594 (14)	0.11988 (12)	0.0227 (5)	
H33	0.5021	0.6975	0.1524	0.027*	
C34	0.54349 (13)	0.74485 (15)	0.08441 (11)	0.0231 (5)	
H34	0.5878	0.7300	0.0927	0.028*	
C35	0.46985 (14)	0.80629 (16)	0.02486 (11)	0.0251 (5)	
H35	0.4628	0.8338	−0.0086	0.030*	
C36	0.41688 (14)	0.79004 (16)	0.05877 (12)	0.0242 (5)	
H36	0.3735	0.8065	0.0492	0.029*	
C37	0.42670 (13)	0.74846 (14)	0.10856 (10)	0.0199 (5)	
C38	0.38690 (17)	0.68721 (18)	0.19277 (14)	0.0374 (7)	
H38A	0.4021	0.6403	0.1806	0.045*	
H38B	0.3451	0.6826	0.2142	0.045*	
H38C	0.4209	0.7089	0.2172	0.045*	
C39	0.30806 (14)	0.7547 (2)	0.12963 (15)	0.0341 (7)	
H39A	0.3072	0.8064	0.1264	0.041*	
H39B	0.2777	0.7397	0.1602	0.041*	
H39C	0.2937	0.7337	0.0934	0.041*	
S3	0.76027 (15)	0.55120 (13)	0.26924 (11)	0.0207 (5)	0.668 (4)
C17	0.8112 (8)	0.4800 (7)	0.2609 (5)	0.021 (3)	0.668 (4)
H17	0.8333	0.4683	0.2263	0.025*	0.668 (4)

C18	0.8162 (7)	0.4416 (8)	0.3103 (5)	0.022 (2)	0.668 (4)
H18	0.8384	0.3974	0.3127	0.026*	0.668 (4)
C19	0.7845 (7)	0.4749 (6)	0.3580 (5)	0.0195 (18)	0.668 (4)
H19	0.7870	0.4585	0.3963	0.023*	0.668 (4)
C20	0.74887 (11)	0.53566 (11)	0.34022 (8)	0.0169 (5)	0.668 (4)
S4	0.41641 (14)	0.8617 (2)	0.25791 (17)	0.0364 (8)	0.656 (5)
C25	0.3827 (7)	0.9126 (9)	0.2054 (5)	0.032 (3)	0.656 (5)
H25	0.3361	0.9218	0.2045	0.039*	0.656 (5)
C26	0.4241 (5)	0.9401 (11)	0.1645 (7)	0.033 (3)	0.656 (5)
H26	0.4135	0.9747	0.1364	0.039*	0.656 (5)
C27	0.4867 (5)	0.9055 (8)	0.1732 (4)	0.031 (3)	0.656 (5)
H27	0.5228	0.9101	0.1472	0.037*	0.656 (5)
C28	0.4912 (6)	0.864 (2)	0.2234 (13)	0.0240 (17)	0.656 (5)
F4	0.7630 (6)	0.8826 (11)	0.4694 (7)	0.025 (2)	0.50
F5	0.7102 (15)	0.8890 (16)	0.5472 (8)	0.085 (4)	0.50
F6	0.738 (8)	0.792 (5)	0.522 (8)	0.0916 (12)	0.50
F10	0.7128 (4)	0.7831 (6)	0.14554 (14)	0.045 (2)	0.472 (7)
F11	0.7484 (3)	0.7097 (2)	0.2073 (3)	0.0290 (12)	0.472 (7)
F12	0.7734 (3)	0.8167 (4)	0.2210 (4)	0.0457 (18)	0.472 (7)
S3'	0.7835 (4)	0.4610 (3)	0.3669 (3)	0.0217 (11)	0.332 (4)
C17'	0.8212 (15)	0.4430 (17)	0.3035 (6)	0.030 (7)	0.332 (4)
H17'	0.8537	0.4071	0.2977	0.036*	0.332 (4)
C18'	0.7980 (17)	0.4876 (16)	0.2619 (10)	0.022 (3)	0.332 (4)
H18'	0.8033	0.4779	0.2224	0.026*	0.332 (4)
C19'	0.7653 (14)	0.5498 (12)	0.2824 (4)	0.042 (8)	0.332 (4)
H19'	0.7564	0.5919	0.2615	0.050*	0.332 (4)
C20'	0.74887 (11)	0.53566 (11)	0.34022 (8)	0.0169 (5)	0.332 (4)
S4'	0.4999 (3)	0.9122 (4)	0.1631 (3)	0.0231 (10)	0.344 (5)
C25'	0.4167 (5)	0.929 (2)	0.1690 (14)	0.032 (6)	0.344 (5)
H25'	0.3939	0.9483	0.1371	0.038*	0.344 (5)
C26'	0.3811 (14)	0.9151 (17)	0.2177 (10)	0.031 (4)	0.344 (5)
H26'	0.3388	0.9326	0.2294	0.037*	0.344 (5)
C27'	0.4254 (7)	0.8673 (10)	0.2461 (10)	0.027 (5)	0.344 (5)
H27'	0.4123	0.8416	0.2791	0.033*	0.344 (5)
C28'	0.4902 (11)	0.861 (4)	0.222 (3)	0.0240 (17)	0.344 (5)
F4'	0.7693 (6)	0.8701 (11)	0.4706 (7)	0.037 (4)	0.50
F5'	0.6989 (15)	0.9023 (15)	0.5362 (9)	0.085 (4)	0.50
F6'	0.738 (8)	0.792 (5)	0.522 (8)	0.0916 (12)	0.50
F10A	0.7067 (9)	0.7574 (9)	0.1485 (3)	0.045 (2)	0.274 (5)
F11A	0.7679 (5)	0.7273 (5)	0.2187 (4)	0.0290 (12)	0.274 (5)
F12A	0.7570 (6)	0.8368 (4)	0.1960 (6)	0.0457 (18)	0.274 (5)
F10B	0.7361 (11)	0.8384 (5)	0.1770 (10)	0.0447 (4)	0.099 (5)
F11B	0.7135 (8)	0.7314 (9)	0.1580 (6)	0.0290 (12)	0.099 (5)
F12B	0.7814 (6)	0.7573 (14)	0.2261 (7)	0.0457 (18)	0.099 (5)
F10C	0.7226 (11)	0.8152 (12)	0.1542 (7)	0.045 (2)	0.156 (7)
F11C	0.7331 (8)	0.7072 (3)	0.1903 (7)	0.0290 (12)	0.156 (7)
F12C	0.7822 (6)	0.7938 (14)	0.2251 (10)	0.0457 (18)	0.156 (7)
H1N	0.5629 (19)	0.798 (2)	0.0139 (16)	0.036 (9)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Eu	0.01078 (8)	0.01810 (8)	0.01641 (8)	0.00051 (4)	0.00067 (4)	−0.00262 (4)
S1	0.0312 (4)	0.0349 (4)	0.0261 (3)	0.0025 (3)	0.0008 (3)	−0.0050 (3)
S2	0.0327 (4)	0.0486 (6)	0.0705 (7)	0.0121 (4)	0.0194 (4)	0.0144 (5)
F1	0.0613 (14)	0.0929 (19)	0.0240 (9)	−0.0511 (13)	0.0071 (9)	−0.0015 (10)
F2	0.0443 (13)	0.143 (3)	0.0381 (11)	−0.0603 (16)	0.0124 (10)	−0.0339 (14)
F3	0.0276 (11)	0.102 (2)	0.091 (2)	0.0076 (13)	0.0156 (12)	−0.0096 (17)
F7	0.0346 (10)	0.0516 (12)	0.0353 (10)	0.0055 (9)	0.0185 (8)	0.0140 (9)
F8	0.0487 (11)	0.0538 (12)	0.0182 (8)	0.0156 (9)	−0.0056 (7)	−0.0067 (8)
F9	0.0433 (11)	0.0482 (12)	0.0254 (8)	0.0211 (9)	0.0091 (7)	0.0135 (8)
O1	0.0211 (9)	0.0323 (11)	0.0275 (10)	−0.0061 (8)	0.0037 (8)	−0.0129 (8)
O2	0.0188 (9)	0.0296 (10)	0.0200 (8)	−0.0077 (7)	−0.0003 (7)	−0.0015 (7)
O3	0.0203 (9)	0.0272 (10)	0.0222 (9)	0.0053 (8)	0.0034 (7)	−0.0040 (7)
O4	0.0201 (9)	0.0260 (10)	0.0199 (8)	−0.0049 (7)	0.0025 (7)	−0.0060 (7)
O5	0.0227 (9)	0.0206 (9)	0.0213 (8)	0.0063 (7)	0.0064 (7)	0.0032 (7)
O6	0.0154 (8)	0.0259 (9)	0.0186 (8)	0.0041 (7)	0.0020 (7)	−0.0014 (7)
O7	0.0176 (9)	0.0365 (11)	0.0186 (9)	0.0092 (8)	−0.0017 (7)	−0.0015 (8)
O8	0.0135 (8)	0.0209 (9)	0.0173 (8)	−0.0008 (7)	−0.0029 (6)	0.0009 (7)
N1	0.0189 (11)	0.0314 (13)	0.0182 (10)	−0.0043 (9)	0.0057 (9)	−0.0001 (9)
N2	0.0202 (12)	0.0327 (13)	0.0299 (13)	−0.0003 (10)	0.0084 (9)	0.0018 (10)
C1	0.060 (2)	0.043 (2)	0.0259 (15)	0.0079 (17)	0.0065 (15)	−0.0089 (14)
C2	0.072 (3)	0.045 (2)	0.0353 (18)	−0.017 (2)	−0.0010 (17)	−0.0150 (15)
C3	0.0364 (15)	0.0262 (14)	0.0215 (12)	−0.0120 (12)	−0.0059 (11)	−0.0002 (10)
C4	0.0313 (14)	0.0242 (13)	0.0181 (12)	0.0016 (11)	−0.0064 (10)	−0.0005 (10)
C5	0.0243 (13)	0.0204 (12)	0.0208 (12)	0.0012 (10)	−0.0073 (10)	−0.0001 (9)
C6	0.0257 (13)	0.0363 (16)	0.0198 (12)	−0.0111 (12)	−0.0066 (10)	−0.0002 (11)
C7	0.0225 (13)	0.0327 (15)	0.0200 (12)	−0.0090 (11)	−0.0038 (10)	0.0049 (10)
C8	0.0318 (16)	0.068 (3)	0.0276 (15)	−0.0248 (17)	0.0035 (13)	−0.0087 (15)
C9	0.044 (2)	0.063 (3)	0.081 (3)	0.023 (2)	0.035 (2)	0.021 (2)
C10	0.074 (3)	0.053 (3)	0.071 (3)	0.026 (2)	0.049 (3)	0.005 (2)
C11	0.0384 (16)	0.0310 (15)	0.0298 (14)	0.0119 (13)	0.0288 (13)	0.0072 (12)
C12	0.0351 (16)	0.0225 (14)	0.0325 (14)	0.0069 (12)	0.0168 (12)	0.0036 (11)
C13	0.0294 (14)	0.0174 (12)	0.0226 (12)	0.0029 (10)	0.0117 (10)	0.0027 (9)
C14	0.0349 (15)	0.0243 (14)	0.0246 (13)	−0.0074 (11)	0.0131 (11)	−0.0071 (11)
C15	0.0278 (14)	0.0260 (14)	0.0192 (12)	−0.0108 (11)	0.0049 (10)	−0.0029 (10)
C16	0.0389 (17)	0.0465 (19)	0.0199 (13)	−0.0188 (14)	0.0010 (12)	−0.0048 (12)
C21	0.0121 (10)	0.0171 (11)	0.0216 (11)	−0.0004 (9)	0.0009 (9)	−0.0032 (9)
C22	0.0184 (12)	0.0211 (12)	0.0199 (11)	0.0022 (9)	0.0023 (9)	0.0010 (9)
C23	0.0161 (11)	0.0238 (13)	0.0169 (11)	−0.0020 (9)	0.0008 (9)	0.0007 (9)
C24	0.0283 (14)	0.0357 (16)	0.0202 (12)	0.0087 (12)	0.0052 (10)	0.0045 (11)
C29	0.0178 (12)	0.0251 (13)	0.0187 (11)	0.0061 (10)	−0.0071 (9)	−0.0064 (10)
C30	0.0196 (12)	0.0308 (14)	0.0147 (11)	0.0054 (10)	−0.0045 (9)	−0.0029 (10)
C31	0.0146 (11)	0.0222 (12)	0.0166 (11)	0.0009 (9)	−0.0018 (9)	−0.0034 (9)
C32	0.0163 (12)	0.0425 (17)	0.0214 (13)	0.0063 (11)	−0.0006 (10)	0.0003 (11)
C33	0.0207 (13)	0.0273 (14)	0.0201 (12)	0.0035 (10)	0.0019 (10)	0.0024 (10)

C34	0.0158 (12)	0.0316 (14)	0.0217 (12)	0.0014 (10)	0.0007 (9)	−0.0029 (10)
C35	0.0271 (13)	0.0303 (14)	0.0178 (11)	0.0012 (11)	−0.0003 (10)	0.0017 (10)
C36	0.0181 (12)	0.0303 (14)	0.0244 (13)	0.0025 (11)	−0.0018 (10)	0.0011 (11)
C37	0.0165 (12)	0.0227 (13)	0.0204 (12)	−0.0014 (9)	0.0030 (9)	−0.0012 (10)
C38	0.0379 (17)	0.0353 (17)	0.0391 (17)	0.0011 (14)	0.0202 (14)	0.0118 (13)
C39	0.0142 (13)	0.0458 (19)	0.0422 (17)	−0.0004 (13)	0.0076 (12)	−0.0040 (14)
S3	0.0214 (9)	0.0209 (7)	0.0198 (7)	−0.0003 (5)	0.0043 (7)	−0.0022 (5)
C17	0.014 (7)	0.023 (3)	0.027 (3)	0.001 (3)	0.011 (3)	−0.005 (2)
C18	0.017 (4)	0.017 (4)	0.031 (3)	0.005 (3)	0.003 (3)	0.006 (3)
C19	0.020 (3)	0.013 (4)	0.025 (4)	−0.003 (3)	0.006 (3)	−0.003 (2)
C20	0.0157 (11)	0.0171 (12)	0.0178 (11)	−0.0011 (9)	0.0022 (9)	−0.0018 (9)
S4	0.0205 (7)	0.0557 (16)	0.0331 (13)	0.0192 (9)	−0.0067 (8)	−0.0065 (9)
C25	0.029 (4)	0.050 (5)	0.019 (5)	0.026 (3)	−0.010 (3)	−0.010 (4)
C26	0.039 (4)	0.034 (7)	0.025 (4)	0.009 (4)	−0.007 (3)	0.000 (3)
C27	0.017 (4)	0.045 (6)	0.031 (6)	0.013 (4)	−0.003 (3)	−0.017 (3)
C28	0.0202 (13)	0.032 (4)	0.0197 (18)	0.0102 (15)	−0.0070 (12)	−0.007 (2)
F4	0.013 (3)	0.031 (5)	0.031 (3)	−0.008 (4)	−0.006 (2)	0.005 (3)
F5	0.030 (8)	0.165 (9)	0.061 (6)	−0.020 (4)	−0.003 (4)	−0.081 (7)
F6	0.108 (2)	0.084 (2)	0.0825 (19)	−0.0538 (18)	−0.0709 (19)	0.0522 (16)
F10	0.035 (3)	0.086 (7)	0.0133 (11)	0.030 (5)	0.0074 (11)	0.016 (2)
F11	0.019 (3)	0.0490 (19)	0.019 (3)	0.0160 (17)	−0.0099 (17)	−0.0033 (16)
F12	0.0167 (19)	0.061 (4)	0.060 (3)	−0.011 (2)	0.0093 (17)	−0.018 (3)
S3'	0.0210 (16)	0.017 (2)	0.027 (2)	0.0032 (17)	−0.0002 (13)	−0.0028 (13)
C17'	0.025 (9)	0.027 (12)	0.038 (10)	−0.002 (7)	0.019 (7)	−0.021 (8)
C18'	0.007 (10)	0.041 (9)	0.018 (6)	−0.006 (5)	0.004 (4)	−0.006 (6)
C19'	0.029 (7)	0.039 (10)	0.058 (15)	0.011 (6)	−0.016 (9)	−0.030 (9)
C20'	0.0157 (11)	0.0171 (12)	0.0178 (11)	−0.0011 (9)	0.0022 (9)	−0.0018 (9)
S4'	0.018 (2)	0.0314 (14)	0.0198 (16)	0.0093 (14)	−0.0012 (15)	−0.0003 (11)
C25'	0.030 (8)	0.033 (11)	0.033 (11)	0.010 (7)	−0.019 (7)	0.006 (6)
C26'	0.032 (7)	0.045 (8)	0.017 (8)	0.009 (6)	−0.002 (6)	−0.012 (7)
C27'	0.037 (9)	0.009 (5)	0.035 (11)	−0.003 (5)	−0.009 (6)	−0.005 (5)
C28'	0.0202 (13)	0.032 (4)	0.0197 (18)	0.0102 (15)	−0.0070 (12)	−0.007 (2)
F4'	0.027 (4)	0.051 (9)	0.032 (4)	0.010 (3)	−0.003 (3)	−0.004 (4)
F5'	0.030 (8)	0.165 (9)	0.061 (6)	−0.020 (4)	−0.003 (4)	−0.081 (7)
F6'	0.108 (2)	0.084 (2)	0.0825 (19)	−0.0538 (18)	−0.0709 (19)	0.0522 (16)
F10A	0.035 (3)	0.086 (7)	0.0133 (11)	0.030 (5)	0.0074 (11)	0.016 (2)
F11A	0.019 (3)	0.0490 (19)	0.019 (3)	0.0160 (17)	−0.0099 (17)	−0.0033 (16)
F12A	0.0167 (19)	0.061 (4)	0.060 (3)	−0.011 (2)	0.0093 (17)	−0.018 (3)
F10B	0.0349 (5)	0.0858 (5)	0.0133 (4)	0.0300 (6)	0.0074 (4)	0.0159 (6)
F11B	0.019 (3)	0.0490 (19)	0.019 (3)	0.0160 (17)	−0.0099 (17)	−0.0033 (16)
F12B	0.0167 (19)	0.061 (4)	0.060 (3)	−0.011 (2)	0.0093 (17)	−0.018 (3)
F10C	0.035 (3)	0.086 (7)	0.0133 (11)	0.030 (5)	0.0074 (11)	0.016 (2)
F11C	0.019 (3)	0.0490 (19)	0.019 (3)	0.0160 (17)	−0.0099 (17)	−0.0033 (16)
F12C	0.0167 (19)	0.061 (4)	0.060 (3)	−0.011 (2)	0.0093 (17)	−0.018 (3)

Geometric parameters (Å, °)

Eu—O2	2.3594 (18)	C23—C24	1.537 (3)
Eu—O3	2.3639 (18)	C29—C30	1.419 (4)

Eu—O8	2.3642 (17)	C29—C28	1.4700 (19)
Eu—O5	2.3810 (18)	C29—C28'	1.470 (2)
Eu—O7	2.3885 (19)	C30—C31	1.381 (3)
Eu—O1	2.3935 (18)	C30—H30	0.9500
Eu—O4	2.4135 (18)	C31—C32	1.537 (3)
Eu—O6	2.4896 (18)	C32—F12B	1.327 (3)
S1—C1	1.703 (4)	C32—F11A	1.327 (3)
S1—C4	1.708 (3)	C32—F10A	1.328 (3)
S2—C9	1.655 (4)	C32—F12C	1.330 (3)
S2—C12	1.704 (4)	C32—F10	1.330 (3)
F1—C8	1.330 (2)	C32—F11B	1.330 (3)
F2—C8	1.327 (2)	C32—F10C	1.331 (3)
F3—C8	1.331 (3)	C32—F11C	1.331 (3)
F7—C24	1.335 (2)	C32—F12A	1.333 (3)
F8—C24	1.335 (2)	C32—F12	1.334 (3)
F9—C24	1.331 (2)	C32—F10B	1.334 (3)
O1—C5	1.250 (3)	C32—F11	1.344 (3)
O2—C7	1.264 (3)	C33—C34	1.356 (4)
O3—C13	1.254 (3)	C33—C37	1.419 (4)
O4—C15	1.265 (3)	C33—H33	0.9500
O5—C21	1.251 (3)	C34—H34	0.9500
O6—C23	1.271 (3)	C35—C36	1.360 (4)
O7—C29	1.258 (3)	C35—H35	0.9500
O8—C31	1.262 (3)	C36—C37	1.420 (4)
N1—C35	1.343 (4)	C36—H36	0.9500
N1—C34	1.348 (4)	C38—H38A	0.9800
N1—H1N	0.87 (4)	C38—H38B	0.9800
N2—C37	1.335 (3)	C38—H38C	0.9800
N2—C38	1.453 (4)	C39—H39A	0.9800
N2—C39	1.462 (4)	C39—H39B	0.9800
C1—C2	1.354 (6)	C39—H39C	0.9800
C1—H1	0.9500	S3—C17	1.700 (3)
C2—C3	1.374 (5)	S3—C20	1.703 (2)
C2—H2	0.9500	C17—C18	1.369 (3)
C3—C4	1.415 (4)	C17—H17	0.9500
C3—H3	0.9500	C18—C19	1.429 (3)
C4—C5	1.460 (4)	C18—H18	0.9500
C5—C6	1.422 (4)	C19—C20	1.416 (3)
C6—C7	1.368 (4)	C19—H19	0.9500
C6—H6	0.9500	S4—C25	1.701 (3)
C7—C8	1.539 (4)	S4—C28	1.702 (3)
C9—C10	1.346 (7)	C25—C26	1.369 (3)
C9—H9	0.9500	C25—H25	0.9500
C10—C11	1.457 (6)	C26—C27	1.429 (3)
C10—H10	0.9500	C26—H26	0.9500
C11—C12	1.507 (4)	C27—C28	1.418 (3)
C11—H11	0.9500	C27—H27	0.9500
C12—C13	1.468 (4)	S3'—C17'	1.699 (3)
C13—C14	1.407 (4)	C17'—C18'	1.369 (3)

C14—C15	1.383 (4)	C17'—H17'	0.9500
C14—H14	0.9500	C18'—C19'	1.430 (3)
C15—C16	1.539 (4)	C18'—H18'	0.9500
C16—F4'	1.328 (3)	C19'—H19'	0.9500
C16—F4	1.329 (3)	S4'—C28'	1.699 (3)
C16—F5	1.329 (3)	S4'—C25'	1.699 (3)
C16—F5'	1.329 (3)	C25'—C26'	1.369 (3)
C16—F6'	1.330 (3)	C25'—H25'	0.9500
C16—F6	1.330 (3)	C26'—C27'	1.430 (3)
C21—C22	1.422 (3)	C26'—H26'	0.9500
C21—C20	1.4694 (13)	C27'—C28'	1.421 (3)
C22—C23	1.376 (3)	C27'—H27'	0.9500
C22—H22	0.9500		
O2—Eu—O3	71.96 (7)	F12B—C32—F11A	28.5 (10)
O2—Eu—O8	146.80 (6)	F12B—C32—F10A	124.8 (11)
O3—Eu—O8	122.74 (6)	F11A—C32—F10A	106.4 (7)
O2—Eu—O5	108.35 (7)	F12B—C32—F12C	30.2 (13)
O3—Eu—O5	153.38 (6)	F11A—C32—F12C	58.6 (12)
O8—Eu—O5	72.17 (6)	F10A—C32—F12C	133.7 (13)
O2—Eu—O7	89.32 (7)	F12B—C32—F10	127.5 (9)
O3—Eu—O7	71.24 (7)	F11A—C32—F10	119.3 (5)
O8—Eu—O7	71.04 (6)	F10A—C32—F10	21.9 (8)
O5—Eu—O7	134.78 (6)	F12C—C32—F10	122.5 (13)
O2—Eu—O1	71.34 (6)	F12B—C32—F11B	108.1 (7)
O3—Eu—O1	130.78 (7)	F11A—C32—F11B	84.7 (7)
O8—Eu—O1	78.07 (6)	F10A—C32—F11B	24.2 (9)
O5—Eu—O1	70.77 (7)	F12C—C32—F11B	128.7 (13)
O7—Eu—O1	76.67 (7)	F10—C32—F11B	45.1 (8)
O2—Eu—O4	131.75 (6)	F12B—C32—F10C	122.4 (13)
O3—Eu—O4	70.25 (7)	F11A—C32—F10C	131.4 (10)
O8—Eu—O4	80.37 (6)	F10A—C32—F10C	51.1 (12)
O5—Eu—O4	93.22 (7)	F12C—C32—F10C	103.2 (16)
O7—Eu—O4	105.52 (7)	F10—C32—F10C	29.2 (10)
O1—Eu—O4	156.25 (6)	F11B—C32—F10C	73.8 (12)
O2—Eu—O6	74.75 (6)	F12B—C32—F11C	73.6 (12)
O3—Eu—O6	85.02 (6)	F11A—C32—F11C	45.8 (8)
O8—Eu—O6	131.75 (6)	F10A—C32—F11C	66.7 (9)
O5—Eu—O6	69.94 (6)	F12C—C32—F11C	102.6 (12)
O7—Eu—O6	154.71 (6)	F10—C32—F11C	86.4 (7)
O1—Eu—O6	115.04 (7)	F11B—C32—F11C	42.6 (10)
O4—Eu—O6	73.15 (6)	F10C—C32—F11C	113.1 (11)
C1—S1—C4	91.91 (16)	F12B—C32—F12A	81.3 (9)
C9—S2—C12	92.7 (2)	F11A—C32—F12A	107.9 (5)
C5—O1—Eu	137.88 (18)	F10A—C32—F12A	105.8 (7)
C7—O2—Eu	134.49 (17)	F12C—C32—F12A	52.4 (13)
C13—O3—Eu	140.66 (18)	F10—C32—F12A	84.6 (7)
C15—O4—Eu	132.68 (17)	F11B—C32—F12A	123.9 (9)
C21—O5—Eu	139.92 (15)	F10C—C32—F12A	56.7 (13)
C23—O6—Eu	132.25 (15)	F11C—C32—F12A	139.7 (8)

C29—O7—Eu	136.81 (16)	F12B—C32—F12	50.8 (10)
C31—O8—Eu	132.00 (16)	F11A—C32—F12	79.2 (5)
C35—N1—C34	120.7 (2)	F10A—C32—F12	132.2 (9)
C35—N1—H1N	115 (2)	F12C—C32—F12	20.7 (11)
C34—N1—H1N	124 (2)	F10—C32—F12	114.1 (5)
C37—N2—C38	120.5 (3)	F11B—C32—F12	138.8 (8)
C37—N2—C39	120.4 (2)	F10C—C32—F12	88.9 (12)
C38—N2—C39	119.0 (2)	F11C—C32—F12	122.5 (7)
C2—C1—S1	112.2 (3)	F12A—C32—F12	33.6 (6)
C2—C1—H1	123.9	F12B—C32—F10B	105.7 (8)
S1—C1—H1	123.9	F11A—C32—F10B	129.0 (9)
C1—C2—C3	113.5 (3)	F10A—C32—F10B	83.4 (9)
C1—C2—H2	123.2	F12C—C32—F10B	78.4 (15)
C3—C2—H2	123.2	F10—C32—F10B	61.4 (11)
C2—C3—C4	112.3 (3)	F11B—C32—F10B	105.4 (8)
C2—C3—H3	123.9	F10C—C32—F10B	32.3 (11)
C4—C3—H3	123.9	F11C—C32—F10B	139.5 (11)
C3—C4—C5	130.5 (3)	F12A—C32—F10B	26.5 (9)
C3—C4—S1	110.1 (2)	F12—C32—F10B	60.2 (11)
C5—C4—S1	119.4 (2)	F12B—C32—F11	53.3 (11)
O1—C5—C6	123.8 (2)	F11A—C32—F11	24.9 (4)
O1—C5—C4	117.6 (2)	F10A—C32—F11	87.4 (7)
C6—C5—C4	118.6 (2)	F12C—C32—F11	83.3 (12)
C7—C6—C5	122.0 (2)	F10—C32—F11	105.4 (4)
C7—C6—H6	119.0	F11B—C32—F11	63.7 (8)
C5—C6—H6	119.0	F10C—C32—F11	128.3 (10)
O2—C7—C6	128.8 (3)	F11C—C32—F11	21.8 (6)
O2—C7—C8	112.5 (2)	F12A—C32—F11	129.8 (5)
C6—C7—C8	118.7 (2)	F12—C32—F11	103.9 (4)
F2—C8—F1	106.7 (2)	F10B—C32—F11	143.9 (8)
F2—C8—F3	107.5 (3)	C34—C33—C37	120.2 (2)
F1—C8—F3	106.3 (3)	C34—C33—H33	119.9
F2—C8—C7	113.8 (2)	C37—C33—H33	119.9
F1—C8—C7	110.9 (2)	N1—C34—C33	121.1 (2)
F3—C8—C7	111.3 (2)	N1—C34—H34	119.5
C10—C9—S2	113.7 (3)	C33—C34—H34	119.5
C10—C9—H9	123.2	N1—C35—C36	121.5 (3)
S2—C9—H9	123.2	N1—C35—H35	119.2
C9—C10—C11	117.0 (3)	C36—C35—H35	119.2
C9—C10—H10	121.5	C35—C36—C37	119.8 (3)
C11—C10—H10	121.5	C35—C36—H36	120.1
C10—C11—C12	103.4 (3)	C37—C36—H36	120.1
C10—C11—H11	128.3	N2—C37—C33	121.8 (2)
C12—C11—H11	128.3	N2—C37—C36	121.5 (3)
C13—C12—C11	128.6 (3)	C33—C37—C36	116.7 (2)
C13—C12—S2	118.3 (2)	N2—C38—H38A	109.5
C11—C12—S2	113.1 (2)	N2—C38—H38B	109.5
O3—C13—C14	123.2 (2)	H38A—C38—H38B	109.5
O3—C13—C12	116.0 (3)	N2—C38—H38C	109.5

C14—C13—C12	120.7 (2)	H38A—C38—H38C	109.5
C15—C14—C13	121.6 (3)	H38B—C38—H38C	109.5
C15—C14—H14	119.2	N2—C39—H39A	109.5
C13—C14—H14	119.2	N2—C39—H39B	109.5
O4—C15—C14	129.0 (3)	H39A—C39—H39B	109.5
O4—C15—C16	113.4 (2)	N2—C39—H39C	109.5
C14—C15—C16	117.5 (2)	H39A—C39—H39C	109.5
F4'—C16—F4	11.6 (19)	H39B—C39—H39C	109.5
F4'—C16—F5	110 (2)	C17—S3—C20	93.2 (4)
F4—C16—F5	105 (2)	C18—C17—S3	111.6 (7)
F4'—C16—F5'	110 (2)	C18—C17—H17	124.2
F4—C16—F5'	101 (2)	S3—C17—H17	124.2
F5—C16—F5'	18.4 (18)	C17—C18—C19	113.2 (9)
F4'—C16—F6'	98 (8)	C17—C18—H18	123.4
F4—C16—F6'	109 (8)	C19—C18—H18	123.4
F5—C16—F6'	98 (9)	C20—C19—C18	110.6 (7)
F5'—C16—F6'	116 (9)	C20—C19—H19	124.7
F4'—C16—F6	98 (8)	C18—C19—H19	124.7
F4—C16—F6	109 (8)	C19—C20—C21	128.6 (5)
F5—C16—F6	98 (9)	C19—C20—S3	111.0 (5)
F5'—C16—F6	116 (9)	C21—C20—S3	120.33 (18)
F6'—C16—F6	0(10)	C25—S4—C28	89.6 (5)
F4'—C16—C15	114.6 (9)	C26—C25—S4	118.8 (11)
F4—C16—C15	111.1 (8)	C26—C25—H25	120.6
F5—C16—C15	121.2 (11)	S4—C25—H25	120.6
F5'—C16—C15	107.8 (10)	C25—C26—C27	104.8 (13)
F6'—C16—C15	111 (7)	C25—C26—H26	127.6
F6—C16—C15	111 (7)	C27—C26—H26	127.6
O5—C21—C22	123.66 (19)	C28—C27—C26	115.5 (10)
O5—C21—C20	117.0 (2)	C28—C27—H27	122.2
C22—C21—C20	119.3 (2)	C26—C27—H27	122.2
C23—C22—C21	122.3 (2)	C27—C28—C29	131.7 (6)
C23—C22—H22	118.9	C27—C28—S4	110.4 (5)
C21—C22—H22	118.9	C29—C28—S4	117.8 (3)
O6—C23—C22	129.5 (2)	C18'—C17'—S3'	110.3 (15)
O6—C23—C24	113.7 (2)	C18'—C17'—H17'	124.9
C22—C23—C24	116.8 (2)	S3'—C17'—H17'	124.9
F9—C24—F7	107.9 (2)	C17'—C18'—C19'	115 (2)
F9—C24—F8	106.9 (2)	C17'—C18'—H18'	122.4
F7—C24—F8	106.9 (2)	C19'—C18'—H18'	122.4
F9—C24—C23	113.80 (19)	C18'—C19'—H19'	127.2
F7—C24—C23	110.72 (19)	C28'—S4'—C25'	85.9 (10)
F8—C24—C23	110.3 (2)	C26'—C25'—S4'	123 (2)
O7—C29—C30	123.9 (2)	C26'—C25'—H25'	118.6
O7—C29—C28	116.9 (5)	S4'—C25'—H25'	118.6
C30—C29—C28	119.2 (5)	C25'—C26'—C27'	101 (2)
O7—C29—C28'	117.2 (10)	C25'—C26'—H26'	129.7
C30—C29—C28'	118.9 (10)	C27'—C26'—H26'	129.7
C28—C29—C28'	3(6)	C28'—C27'—C26'	116 (2)

C31—C30—C29	121.6 (2)	C28'—C27'—H27'	122.1
C31—C30—H30	119.2	C26'—C27'—H27'	122.1
C29—C30—H30	119.2	C27'—C28'—C29	125.5 (12)
O8—C31—C30	128.5 (2)	C27'—C28'—S4'	112.1 (13)
O8—C31—C32	113.6 (2)	C29—C28'—S4'	121.9 (4)
C30—C31—C32	117.8 (2)		
O2—Eu—O1—C5	1.7 (3)	S2—C12—C13—C14	−178.4 (2)
O3—Eu—O1—C5	−42.0 (3)	O3—C13—C14—C15	0.4 (4)
O8—Eu—O1—C5	−165.2 (3)	C12—C13—C14—C15	177.9 (3)
O5—Eu—O1—C5	119.8 (3)	Eu—O4—C15—C14	−21.0 (5)
O7—Eu—O1—C5	−92.1 (3)	Eu—O4—C15—C16	155.28 (17)
O4—Eu—O1—C5	169.6 (2)	C13—C14—C15—O4	8.0 (5)
O6—Eu—O1—C5	64.1 (3)	C13—C14—C15—C16	−168.1 (2)
O3—Eu—O2—C7	133.8 (3)	O4—C15—C16—F4'	45.6 (11)
O8—Eu—O2—C7	11.0 (3)	C14—C15—C16—F4'	−137.7 (11)
O5—Eu—O2—C7	−74.3 (3)	O4—C15—C16—F4	57.6 (10)
O7—Eu—O2—C7	63.3 (3)	C14—C15—C16—F4	−125.7 (11)
O1—Eu—O2—C7	−12.8 (3)	O4—C15—C16—F5	−178 (2)
O4—Eu—O2—C7	173.7 (2)	C14—C15—C16—F5	−2(2)
O6—Eu—O2—C7	−136.5 (3)	O4—C15—C16—F5'	167.9 (18)
O2—Eu—O3—C13	138.9 (3)	C14—C15—C16—F5'	−15.4 (18)
O8—Eu—O3—C13	−74.3 (3)	O4—C15—C16—F6'	−64 (9)
O5—Eu—O3—C13	43.8 (4)	C14—C15—C16—F6'	113 (9)
O7—Eu—O3—C13	−125.5 (3)	O4—C15—C16—F6	−64 (9)
O1—Eu—O3—C13	−177.6 (3)	C14—C15—C16—F6	113 (9)
O4—Eu—O3—C13	−10.5 (3)	Eu—O5—C21—C22	−18.8 (4)
O6—Eu—O3—C13	63.4 (3)	Eu—O5—C21—C20	161.13 (18)
O2—Eu—O4—C15	−23.4 (3)	O5—C21—C22—C23	2.3 (4)
O3—Eu—O4—C15	17.0 (2)	C20—C21—C22—C23	−177.6 (2)
O8—Eu—O4—C15	147.1 (3)	Eu—O6—C23—C22	4.7 (4)
O5—Eu—O4—C15	−141.6 (2)	Eu—O6—C23—C24	−175.31 (14)
O7—Eu—O4—C15	80.0 (3)	C21—C22—C23—O6	3.5 (4)
O1—Eu—O4—C15	172.1 (2)	C21—C22—C23—C24	−176.5 (2)
O6—Eu—O4—C15	−73.7 (2)	O6—C23—C24—F9	−172.8 (2)
O2—Eu—O5—C21	−46.7 (3)	C22—C23—C24—F9	7.1 (3)
O3—Eu—O5—C21	39.5 (3)	O6—C23—C24—F7	65.4 (3)
O8—Eu—O5—C21	168.2 (3)	C22—C23—C24—F7	−114.6 (2)
O7—Eu—O5—C21	−154.9 (2)	O6—C23—C24—F8	−52.7 (3)
O1—Eu—O5—C21	−108.5 (3)	C22—C23—C24—F8	127.3 (2)
O4—Eu—O5—C21	89.4 (3)	Eu—O7—C29—C30	−6.9 (4)
O6—Eu—O5—C21	18.7 (3)	Eu—O7—C29—C28	174 (2)
O2—Eu—O6—C23	106.0 (2)	Eu—O7—C29—C28'	171 (4)
O3—Eu—O6—C23	178.7 (2)	O7—C29—C30—C31	−7.3 (4)
O8—Eu—O6—C23	−50.8 (2)	C28—C29—C30—C31	172 (2)
O5—Eu—O6—C23	−10.5 (2)	C28'—C29—C30—C31	175 (4)
O7—Eu—O6—C23	158.7 (2)	Eu—O8—C31—C30	27.7 (4)
O1—Eu—O6—C23	45.6 (2)	Eu—O8—C31—C32	−154.24 (15)
O4—Eu—O6—C23	−110.5 (2)	C29—C30—C31—O8	−3.4 (4)
O2—Eu—O7—C29	−134.9 (3)	C29—C30—C31—C32	178.7 (2)

O3—Eu—O7—C29	154.0 (3)	C35—N1—C34—C33	0.2 (4)
O8—Eu—O7—C29	17.8 (2)	C37—C33—C34—N1	−0.8 (4)
O5—Eu—O7—C29	−19.3 (3)	C34—N1—C35—C36	0.6 (4)
O1—Eu—O7—C29	−63.9 (3)	N1—C35—C36—C37	−0.6 (4)
O4—Eu—O7—C29	91.7 (3)	C38—N2—C37—C33	−1.6 (4)
O6—Eu—O7—C29	175.0 (2)	C39—N2—C37—C33	−179.2 (3)
O2—Eu—O8—C31	29.9 (3)	C38—N2—C37—C36	178.3 (3)
O3—Eu—O8—C31	−78.2 (2)	C39—N2—C37—C36	0.7 (4)
O5—Eu—O8—C31	126.3 (2)	C34—C33—C37—N2	−179.3 (3)
O7—Eu—O8—C31	−26.9 (2)	C34—C33—C37—C36	0.8 (4)
O1—Eu—O8—C31	52.9 (2)	C35—C36—C37—N2	−180.0 (3)
O4—Eu—O8—C31	−137.1 (2)	C35—C36—C37—C33	−0.1 (4)
O6—Eu—O8—C31	165.9 (2)	C20—S3—C17—C18	4.1 (15)
C4—S1—C1—C2	0.2 (3)	S3—C17—C18—C19	−7(2)
S1—C1—C2—C3	−0.3 (5)	C17—C18—C19—C20	7(2)
C1—C2—C3—C4	0.2 (5)	C18—C19—C20—C21	176.0 (9)
C2—C3—C4—C5	−177.2 (3)	C18—C19—C20—S3	−3.8 (15)
C2—C3—C4—S1	0.0 (4)	O5—C21—C20—C19	174.5 (10)
C1—S1—C4—C3	−0.1 (2)	C22—C21—C20—C19	−5.6 (10)
C1—S1—C4—C5	177.4 (2)	O5—C21—C20—S3	−5.7 (3)
Eu—O1—C5—C6	6.7 (4)	C22—C21—C20—S3	174.2 (2)
Eu—O1—C5—C4	−174.05 (19)	C17—S3—C20—C19	−0.1 (11)
C3—C4—C5—O1	177.2 (3)	C17—S3—C20—C21	−179.9 (7)
S1—C4—C5—O1	0.3 (3)	C28—S4—C25—C26	−7(2)
C3—C4—C5—C6	−3.4 (4)	S4—C25—C26—C27	10 (2)
S1—C4—C5—C6	179.6 (2)	C25—C26—C27—C28	−9(3)
O1—C5—C6—C7	−8.3 (5)	C26—C27—C28—C29	−178 (4)
C4—C5—C6—C7	172.4 (3)	C26—C27—C28—S4	4(4)
Eu—O2—C7—C6	16.2 (5)	O7—C29—C28—C27	171 (4)
Eu—O2—C7—C8	−161.58 (18)	C30—C29—C28—C27	−8(6)
C5—C6—C7—O2	−2.8 (5)	C28'—C29—C28—C27	−92 (22)
C5—C6—C7—C8	174.8 (3)	O7—C29—C28—S4	−11 (4)
O2—C7—C8—F2	−171.5 (3)	C30—C29—C28—S4	170 (2)
C6—C7—C8—F2	10.5 (4)	C28'—C29—C28—S4	86 (15)
O2—C7—C8—F1	−51.2 (3)	C25—S4—C28—C27	1(3)
C6—C7—C8—F1	130.8 (3)	C25—S4—C28—C29	−177 (3)
O2—C7—C8—F3	66.9 (3)	S3'—C17'—C18'—C19'	18 (4)
C6—C7—C8—F3	−111.1 (3)	C28'—S4'—C25'—C26'	16 (5)
C12—S2—C9—C10	0.8 (4)	S4'—C25'—C26'—C27'	−18 (4)
S2—C9—C10—C11	1.2 (5)	C25'—C26'—C27'—C28'	10 (6)
C9—C10—C11—C12	−2.7 (5)	C26'—C27'—C28'—C29	171 (6)
C10—C11—C12—C13	−176.1 (3)	C26'—C27'—C28'—S4'	0(8)
C10—C11—C12—S2	3.2 (3)	O7—C29—C28'—C27'	−5(10)
C9—S2—C12—C13	177.0 (3)	C30—C29—C28'—C27'	173 (6)
C9—S2—C12—C11	−2.5 (3)	C28—C29—C28'—C27'	−89 (24)
Eu—O3—C13—C14	5.4 (4)	O7—C29—C28'—S4'	166 (5)
Eu—O3—C13—C12	−172.08 (19)	C30—C29—C28'—S4'	−16 (9)
C11—C12—C13—O3	178.5 (3)	C28—C29—C28'—S4'	81 (12)
S2—C12—C13—O3	−0.8 (3)	C25'—S4'—C28'—C27'	−8(6)

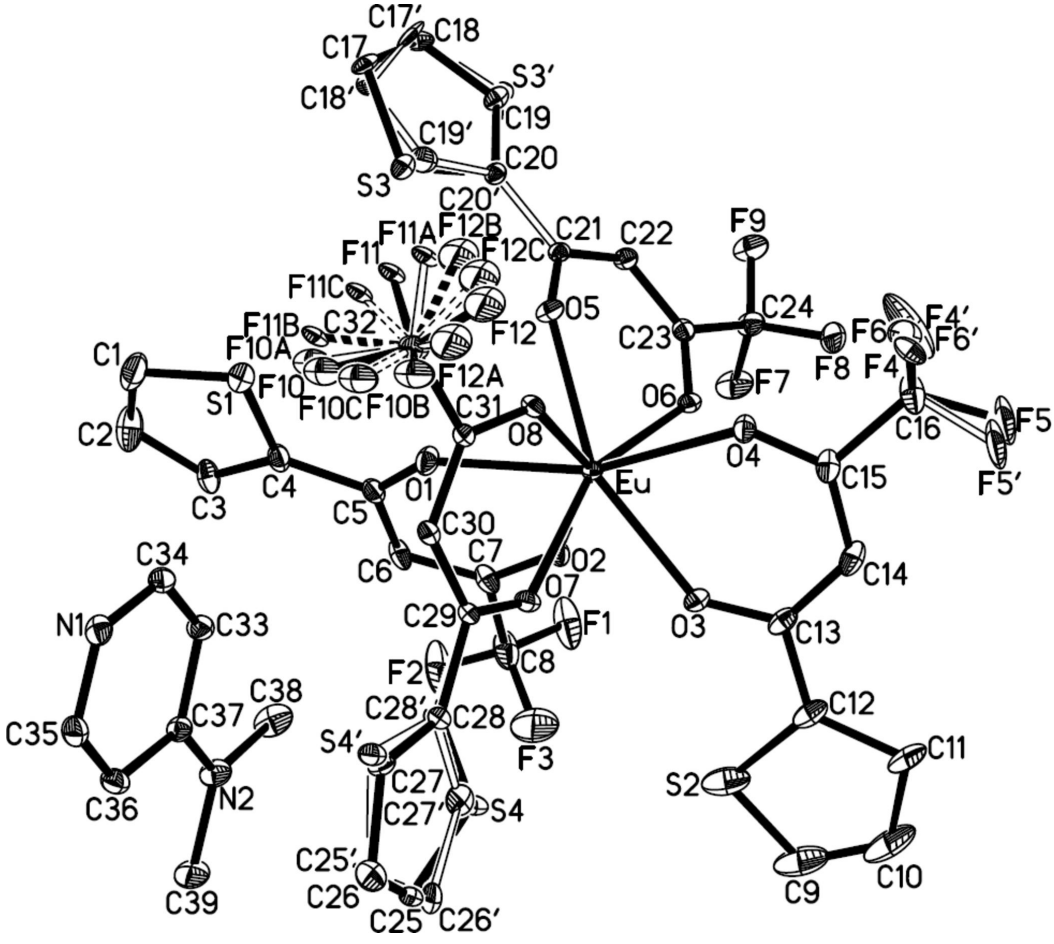
C11—C12—C13—C14	0.9 (4)	C25'—S4'—C28'—C29	−179 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O6^{i}	0.87 (4)	1.96 (4)	2.814 (3)	168 (4)

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2.

Fig. 1


C17′
C18
C17
S3′
C18′
C19
C19′
C20
S3
C20′
F11A
F12B
C21
C22
F9
F11
F12C
F11C
O5
C24
F11B
C32
F12
C23
F6
F4′
F6′
C1
F10A
F8
F4
F10
F12A
O6
F7
S1
F10C
F10B
C31
C16
F5
C2
O8
O4
O1
Eu
C15
F5′
C3
C4
C5
C30
C6
C7
O2
C14
C34
O7
N1
C33
C29
F1
O3
C13
F2
C8
C38
C28′
C28
C12
C35
C37
S4′
F3
C11
C27
S2
N2
C36
C27′
S4
C25′
C10
C26
C9
C39
C25
C26′