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(Bipyridyl-κ^2N,N')bis(η^5-pentamethylcyclopentadienyl)(trifluoromethanesulfonato-κO)cerium(III)

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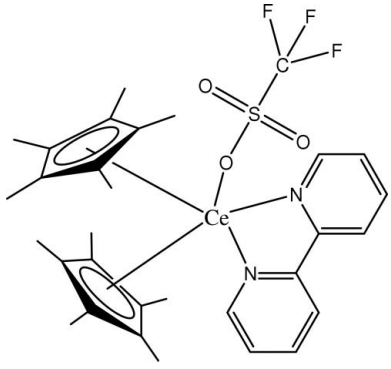
Key indicators: single-crystal X-ray study; T = 140 K; mean σ(C–C) = 0.008 Å; R factor = 0.035; wR factor = 0.041; data-to-parameter ratio = 13.1.

The title compound, $[Ce(CF_3SO_3)(C_{10}H_{15})_2(C_{10}H_8N_2)]$, crystallizes as a bent metallocene with an inner-sphere trifluoromethanesulfonate ligand [$Cg1$—Ce—$Cg2$ = 138.91 (1) Å; $Cg1$ and $Cg2$ are the centroids of the cyclopentadienyl rings]. The pentamethylcyclopentadienyl rings have a slightly staggered conformation. The bipyridine ligand has an N—C—C—N torsion angle of −8.2 (7)°.

Related literature

For related literature, see: Hazin *et al.* (1988); Schultz *et al.* (2002).



Experimental

Crystal data

$[Ce(CF_3O_3S)(C_{10}H_{15})_2(C_{10}H_8N_2)]$
M_r = 715.83
Monoclinic, $P2_1/n$
a = 12.162 (1) Å
b = 15.377 (2) Å
c = 16.132 (1) Å
β = 90.938 (2)°
V = 3016.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.63 mm^{-1}
T = 140.2 K
0.21 × 0.11 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2003; Blessing, 1995)
T_{min} = 0.705, T_{max} = 0.850
13359 measured reflections
4860 independent reflections
3297 reflections with $F^2 > 3\sigma(F^2)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.041
S = 1.38
4860 reflections
370 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −1.12 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ce1—O1	2.649 (3)	Ce1—$Cg1$	2.5382 (3)
Ce1—N1	2.603 (4)	Ce1—$Cg2$	2.5439 (3)
Ce1—N2	2.677 (4)		
O1—Ce1—N1	142.7 (1)	N1—Ce1—N2	61.3 (1)
O1—Ce1—N2	81.5 (1)		

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT* and *XPREP* (Bruker, 2001); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *TEXSAN* (Molecular Structure Corporation, 1998); molecular graphics: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

We thank Drs Fred Hollander and Allen Oliver, Professor Kenneth Raymond, and Bryan Tiedmann.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2372).

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supplementary materials

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(Bipyridyl-κ^2N,N')bis(η^5-pentamethylcyclopentadienyl)(trifluoromethanesulfonato-κO)cerium(III)

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Comment

In the title compound, (η^5-cp*)$_2$Ce(2,2-bipyridine)(OTf), [Cp* is pentamethylcyclopentadienyl and OTf is trifluoromethanesulfonate], the Cp* rings are slightly staggered. Table 1 lists selected bond lengths and angles. The cyclopentadienyl ligands are represented by *Cg*1 and *Cg*2, where *Cg*1 and *Cg*2 are the centroids of the C1—C5 and C6—C10 rings, respectively. The Ce1—*Cg*1 and Ce1—*Cg*2 distances are similar to those observed in (η^5-Cp*)$_2$Ce(CH$_3$CN)$_2$ (2.53 Å; Hazin *et al.*, 1988). The two pyridine rings of the bipyridine ligand are not coplanar. The N1—C25—C26—N2 torsion angle of −8.2 (7)° is not uncommon for neutral bipyridine bound to a lanthanide (Schultz *et al.*, 2002). The trifluoromethanesulfonate anion is bound inner-sphere.

Experimental

(η^5-C$_5$Me$_5$)$_2$Ce(OTf) (1.4 g, 2.4 mmol) and bipy (0.41 g, 2.6 mmol) were mixed in pentane (50 ml) with stirring. After stirring the solution overnight, the resulting yellow-red solution was then filtered and the filtrate was taken to dryness. The product is insoluble in pentane and toluene, and THF displaces the bipy. The product was crystallized by layering pentane onto a concentrated dichloromethane solution and then recrystallized in a similar manner, yielding red crystals (yield 0.58 g, 33%; m.p.: 483–485 K). Analysis calculated for C$_{31}$H$_{38}$CeF$_3$N$_2$O$_3$S: C 52.02, H 5.35, N 3.91; found: C 52.03, H 5.37, N 3.91. The crystal was handled under nitrogen atmosphere, mounted on a glass fiber with Paratone-N oil and cooled to 140 (2) K for data collection.

Refinement

H atoms were placed in calculated positions, with C—H = 0.95–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

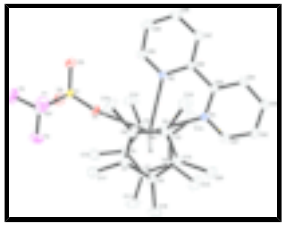


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms have been omitted for clarity.

(Bipyridyl-κ^2*N*,*N*′)bis(η^5-pentamethylcyclopentadienyl) (trifluoromethanesulfonato-κ*O*)cerium(III)

Crystal data

$[Ce(CF_3O_3S_1)(C_{10}H_{15})_2(C_{10}H_8N_2)]$	F_{000} = 1452.00
M_r = 715.83	D_x = 1.576 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point = 483–485 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.7107 Å
a = 12.162 (1) Å	Cell parameters from 4314 reflections
b = 15.377 (2) Å	θ = 2.5–24.7º
c = 16.132 (1) Å	μ = 1.63 mm^{-1}
β = 90.938 (2)º	T = 140.2 K
V = 3016.6 (5) Å^3	Rectangular block, dark brown
Z = 4	0.21 × 0.11 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	3297 reflections with $F^2 > 3\sigma(F^2)$
ω scans	R_{int} = 0.042
Absorption correction: multi-scan (SADABS; Bruker, 2003; Blessing, 1995)	θ_{max} = 24.7º
T_{min} = 0.705, T_{max} = 0.850	h = 0→14
13359 measured reflections	k = 0→17
4860 independent reflections	l = −18→18

Refinement

Refinement on F	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$w = 1/[\sigma^2(F_o) + 0.00022\|F_o\|^2]$
$wR(F^2)$ = 0.041	$(\Delta/\sigma)_{max}$ = 0.0004
S = 1.38	$\Delta\rho_{max}$ = 0.72 e Å^{-3}
4860 reflections	$\Delta\rho_{min}$ = −1.12 e Å^{-3}
370 parameters	Extinction correction: none

Special details

Geometry. no

Refinement. Refinement using reflections with $F^2 > 3.0\ \sigma(F^2)$. The weighted *R*-factor (*wR*), goodness of fit (*S*) and *R*-factor (gt) are based on *F*, with *F* set to zero for negative *F*. The threshold expression of $F^2 > 3.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}

Ce1	0.23757 (2)	0.24695 (2)	0.02756 (2)	0.01241 (8)
S1	0.1044 (1)	0.14345 (9)	−0.18477 (8)	0.0167 (4)
F1	0.1436 (3)	−0.0242 (2)	−0.1591 (2)	0.031 (1)
F2	0.1205 (3)	0.0124 (2)	−0.2862 (2)	0.035 (1)
F3	0.2719 (3)	0.0429 (2)	−0.2222 (2)	0.030 (1)
O1	0.1646 (3)	0.1686 (2)	−0.1088 (2)	0.016 (1)
O2	0.1286 (3)	0.1959 (2)	−0.2561 (2)	0.024 (1)
O3	−0.0092 (3)	0.1232 (2)	−0.1720 (2)	0.024 (1)
N1	0.1725 (3)	0.3264 (3)	0.1606 (3)	0.016 (1)
N2	0.0216 (4)	0.2675 (3)	0.0503 (3)	0.020 (1)
C1	0.4088 (4)	0.3454 (4)	−0.0422 (3)	0.020 (2)
C2	0.3691 (5)	0.3996 (3)	0.0208 (3)	0.021 (2)
C3	0.2612 (5)	0.4267 (3)	−0.0013 (4)	0.019 (2)
C4	0.2343 (5)	0.3885 (4)	−0.0787 (3)	0.020 (2)
C5	0.3260 (5)	0.3388 (3)	−0.1045 (3)	0.019 (2)
C6	0.3959 (4)	0.1369 (3)	0.1037 (3)	0.016 (2)
C7	0.3376 (5)	0.0891 (3)	0.0413 (3)	0.016 (2)
C8	0.2291 (5)	0.0745 (3)	0.0703 (3)	0.017 (2)
C9	0.2203 (4)	0.1134 (3)	0.1498 (3)	0.017 (2)
C10	0.3243 (5)	0.1501 (3)	0.1702 (3)	0.017 (2)
C11	0.5252 (5)	0.3135 (4)	−0.0518 (4)	0.035 (2)
C12	0.4391 (6)	0.4341 (4)	0.0920 (4)	0.036 (2)
C13	0.1903 (6)	0.4916 (4)	0.0417 (4)	0.037 (2)
C14	0.1287 (5)	0.4018 (4)	−0.1287 (4)	0.030 (2)
C15	0.3436 (5)	0.2970 (4)	−0.1873 (4)	0.027 (2)
C16	0.5164 (5)	0.1562 (4)	0.1060 (4)	0.026 (2)
C17	0.3811 (5)	0.0626 (4)	−0.0411 (4)	0.026 (2)
C18	0.1396 (5)	0.0212 (4)	0.0293 (4)	0.029 (2)
C19	0.1235 (5)	0.1100 (4)	0.2046 (4)	0.029 (2)
C20	0.3593 (5)	0.1777 (4)	0.2566 (3)	0.025 (2)
C21	0.2497 (4)	0.3563 (3)	0.2142 (3)	0.018 (2)
C22	0.2264 (5)	0.4076 (4)	0.2821 (3)	0.022 (2)
C23	0.1198 (5)	0.4304 (4)	0.2964 (3)	0.025 (2)
C24	0.0375 (5)	0.3989 (4)	0.2431 (3)	0.022 (2)
C25	0.0667 (4)	0.3470 (3)	0.1758 (3)	0.017 (2)
C26	−0.0168 (4)	0.3092 (3)	0.1180 (3)	0.015 (2)
C27	−0.1290 (5)	0.3157 (4)	0.1323 (3)	0.023 (2)
C28	−0.2033 (5)	0.2773 (4)	0.0781 (4)	0.024 (2)
C29	−0.1645 (5)	0.2348 (4)	0.0096 (4)	0.030 (2)
C30	−0.0525 (5)	0.2314 (4)	−0.0017 (4)	0.028 (2)
C31	0.1636 (5)	0.0382 (4)	−0.2135 (3)	0.022 (2)
H11A	0.5248	0.2581	−0.0775	0.0416*
H11B	0.5602	0.3097	0.0011	0.0416*
H11C	0.5646	0.3536	−0.0854	0.0416*
H12A	0.4683	0.3867	0.1231	0.0447*
H12B	0.4978	0.4677	0.0707	0.0447*
H12C	0.3953	0.4693	0.1267	0.0447*
H13A	0.1223	0.4652	0.0553	0.0452*
H13B	0.2266	0.5107	0.0911	0.0452*

H13C	0.1771	0.5398	0.0063	0.0452*
H14A	0.0682	0.3823	−0.0972	0.0358*
H14B	0.1203	0.4615	−0.1414	0.0358*
H14C	0.1323	0.3690	−0.1786	0.0358*
H15A	0.3637	0.2379	−0.1793	0.0331*
H15B	0.2770	0.2997	−0.2192	0.0331*
H15C	0.3999	0.3268	−0.2154	0.0331*
H16A	0.5528	0.1159	0.1414	0.0316*
H16B	0.5447	0.1515	0.0515	0.0316*
H16C	0.5279	0.2136	0.1261	0.0316*
H17A	0.4183	0.1104	−0.0652	0.0310*
H17B	0.4313	0.0157	−0.0335	0.0310*
H17C	0.3221	0.0449	−0.0761	0.0310*
H18A	0.1716	−0.0273	0.0026	0.0351*
H18B	0.1014	0.0560	−0.0104	0.0351*
H18C	0.0899	0.0017	0.0701	0.0351*
H19A	0.1310	0.0645	0.2448	0.0339*
H19B	0.0571	0.0999	0.1732	0.0339*
H19C	0.1150	0.1639	0.2340	0.0339*
H20A	0.4236	0.2126	0.2535	0.0296*
H20B	0.3020	0.2102	0.2809	0.0296*
H20C	0.3746	0.1276	0.2892	0.0296*
H21	0.3239	0.3416	0.2049	0.0208*
H22	0.2844	0.4263	0.3185	0.0258*
H23	0.1022	0.4664	0.3427	0.0303*
H24	−0.0376	0.4129	0.2525	0.0260*
H27	−0.1542	0.3468	0.1792	0.0277*
H28	−0.2797	0.2798	0.0880	0.0288*
H29	−0.2132	0.2084	−0.0296	0.0358*
H30	−0.0262	0.2021	−0.0491	0.0344*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.0125 (2)	0.0120 (2)	0.0127 (2)	−0.0004 (2)	−0.0016 (1)	0.0009 (2)
S1	0.0177 (8)	0.0176 (8)	0.0146 (8)	0.0002 (6)	−0.0032 (6)	−0.0003 (6)
F1	0.041 (2)	0.020 (2)	0.031 (2)	−0.003 (2)	0.002 (2)	0.003 (2)
F2	0.047 (2)	0.032 (2)	0.025 (2)	0.012 (2)	−0.017 (2)	−0.014 (2)
F3	0.018 (2)	0.036 (2)	0.036 (2)	0.005 (2)	0.005 (2)	−0.003 (2)
O1	0.020 (2)	0.016 (2)	0.014 (2)	−0.001 (2)	−0.006 (2)	−0.002 (2)
O2	0.030 (2)	0.025 (2)	0.017 (2)	−0.002 (2)	−0.002 (2)	0.007 (2)
O3	0.017 (2)	0.030 (2)	0.026 (2)	−0.003 (2)	−0.002 (2)	−0.005 (2)
N1	0.015 (3)	0.017 (3)	0.018 (3)	−0.002 (2)	0.000 (2)	0.000 (2)
N2	0.015 (3)	0.024 (3)	0.021 (3)	0.002 (2)	0.001 (2)	−0.006 (2)
C1	0.020 (3)	0.018 (3)	0.022 (3)	−0.009 (2)	−0.003 (3)	0.004 (3)
C2	0.030 (4)	0.015 (3)	0.017 (3)	−0.016 (3)	−0.002 (3)	0.006 (3)
C3	0.030 (4)	0.011 (3)	0.017 (3)	0.002 (3)	0.002 (3)	0.006 (2)
C4	0.028 (4)	0.017 (3)	0.014 (3)	0.001 (3)	−0.003 (3)	0.011 (2)

C5	0.029 (4)	0.013 (3)	0.016 (3)	−0.003 (2)	0.004 (3)	0.003 (2)
C6	0.016 (3)	0.016 (3)	0.016 (3)	−0.004 (2)	−0.006 (2)	0.006 (2)
C7	0.023 (4)	0.010 (3)	0.016 (3)	0.006 (2)	−0.001 (3)	0.002 (2)
C8	0.023 (3)	0.010 (3)	0.019 (3)	−0.001 (2)	−0.009 (3)	0.006 (2)
C9	0.017 (3)	0.017 (3)	0.017 (3)	−0.003 (2)	0.001 (2)	0.005 (3)
C10	0.024 (3)	0.008 (3)	0.019 (3)	0.002 (2)	−0.004 (3)	0.001 (2)
C11	0.021 (4)	0.046 (4)	0.036 (4)	−0.005 (3)	−0.004 (3)	0.014 (3)
C12	0.048 (5)	0.035 (4)	0.026 (4)	−0.026 (3)	−0.007 (3)	0.007 (3)
C13	0.058 (5)	0.023 (4)	0.030 (4)	0.008 (3)	0.008 (3)	0.009 (3)
C14	0.026 (4)	0.033 (4)	0.031 (4)	0.003 (3)	−0.003 (3)	0.017 (3)
C15	0.027 (4)	0.027 (4)	0.028 (4)	−0.005 (3)	0.006 (3)	−0.002 (3)
C16	0.018 (3)	0.027 (4)	0.034 (4)	0.006 (3)	0.000 (3)	0.001 (3)
C17	0.026 (4)	0.024 (3)	0.026 (4)	0.008 (3)	−0.007 (3)	−0.001 (3)
C18	0.041 (4)	0.019 (3)	0.027 (4)	−0.018 (3)	−0.015 (3)	0.007 (3)
C19	0.029 (4)	0.032 (4)	0.025 (4)	−0.001 (3)	0.001 (3)	0.010 (3)
C20	0.027 (4)	0.024 (3)	0.021 (3)	0.002 (3)	−0.009 (3)	−0.001 (3)
C21	0.020 (3)	0.016 (3)	0.018 (3)	−0.001 (3)	0.002 (3)	0.001 (3)
C22	0.026 (4)	0.020 (3)	0.020 (3)	−0.008 (3)	−0.003 (3)	−0.003 (3)
C23	0.032 (4)	0.023 (3)	0.019 (3)	0.001 (3)	0.004 (3)	−0.011 (3)
C24	0.017 (3)	0.025 (3)	0.022 (3)	0.004 (3)	0.001 (3)	−0.004 (3)
C25	0.018 (3)	0.015 (3)	0.016 (3)	0.003 (2)	0.001 (2)	0.002 (2)
C26	0.017 (3)	0.016 (3)	0.012 (3)	0.000 (2)	0.000 (2)	0.001 (2)
C27	0.025 (4)	0.030 (3)	0.014 (3)	0.004 (3)	0.003 (3)	0.001 (3)
C28	0.016 (3)	0.030 (4)	0.025 (4)	−0.003 (2)	0.001 (3)	0.001 (3)
C29	0.020 (3)	0.039 (4)	0.031 (4)	−0.002 (3)	−0.006 (3)	−0.007 (3)
C30	0.019 (3)	0.040 (4)	0.027 (4)	0.000 (3)	0.001 (3)	−0.014 (3)
C31	0.028 (4)	0.023 (3)	0.014 (3)	0.000 (3)	−0.003 (3)	0.000 (3)

Geometric parameters (Å, °)

Ce1—O1	2.649 (3)	C9—C19	1.485 (8)
Ce1—N1	2.603 (4)	C9—Cg2	1.212 (6)
Ce1—N2	2.677 (4)	C10—C20	1.511 (7)
Ce1—C1	2.823 (5)	C10—Cg2	1.197 (5)
Ce1—C2	2.843 (5)	C21—C22	1.383 (7)
Ce1—C3	2.818 (5)	C22—C23	1.366 (8)
Ce1—C4	2.771 (5)	C23—C24	1.396 (7)
Ce1—C5	2.787 (5)	C24—C25	1.398 (7)
Ce1—C6	2.829 (5)	C25—C26	1.485 (7)
Ce1—C7	2.722 (5)	C26—C27	1.392 (8)
Ce1—C8	2.742 (5)	C27—C28	1.381 (8)
Ce1—C9	2.857 (5)	C28—C29	1.373 (9)
Ce1—Cg1	2.5382 (3)	C29—C30	1.379 (8)
Ce1—Cg2	2.5439 (3)	C11—H11A	0.946
S1—O1	1.468 (4)	C11—H11B	0.950
S1—O2	1.440 (4)	C11—H11C	0.955
S1—O3	1.435 (4)	C12—H12A	0.951
S1—C31	1.833 (6)	C12—H12B	0.951
F1—C31	1.326 (6)	C12—H12C	0.948

F2—C31	1.337 (6)	C13—H13A	0.951
F3—C31	1.329 (7)	C13—H13B	0.951
N1—C21	1.348 (6)	C13—H13C	0.948
N1—C25	1.352 (7)	C14—H14A	0.950
N2—C26	1.355 (7)	C14—H14B	0.946
N2—C30	1.342 (7)	C14—H14C	0.951
C1—C2	1.406 (8)	C15—H15A	0.949
C1—C5	1.414 (7)	C15—H15B	0.954
C1—C11	1.509 (8)	C15—H15C	0.945
C1—Cg1	1.204 (6)	C16—H16A	0.947
C2—C3	1.417 (8)	C16—H16B	0.952
C2—C12	1.514 (8)	C16—H16C	0.949
C2—Cg1	1.197 (5)	C17—H17A	0.950
C3—C4	1.414 (8)	C17—H17B	0.951
C3—C13	1.497 (8)	C17—H17C	0.946
C3—Cg1	1.208 (6)	C18—H18A	0.948
C4—C5	1.420 (8)	C18—H18B	0.950
C4—C14	1.519 (8)	C18—H18C	0.948
C4—Cg1	1.203 (5)	C19—H19A	0.957
C5—C15	1.500 (8)	C19—H19B	0.960
C5—Cg1	1.204 (5)	C19—H19C	0.962
C6—C7	1.426 (7)	C20—H20A	0.950
C6—C10	1.406 (7)	C20—H20B	0.948
C6—C16	1.496 (7)	C20—H20C	0.950
C6—Cg2	1.210 (5)	C21—H21	0.945
C7—C8	1.426 (8)	C22—H22	0.955
C7—C17	1.496 (8)	C23—H23	0.956
C7—Cg2	1.212 (6)	C24—H24	0.953
C8—C9	1.419 (8)	C27—H27	0.949
C8—C18	1.507 (7)	C28—H28	0.947
C8—Cg2	1.206 (5)	C29—H29	0.950
C9—C10	1.419 (7)	C30—H30	0.948
Ce1···O1	2.649 (3)	F2···Cg1^{iii}	3.536 (3)
Ce1···N1	2.603 (4)	F3···C24^{iv}	3.406 (6)
Ce1···N2	2.677 (4)	F3···C27^{iv}	3.431 (7)
Ce1···C1	2.823 (5)	F3···C14^{iii}	3.471 (7)
Ce1···C2	2.843 (5)	O2···C28^{iv}	3.418 (7)
Ce1···C3	2.818 (5)	O2···C16^{ii}	3.447 (7)
Ce1···C4	2.771 (5)	O2···C27^{iv}	3.483 (7)
Ce1···C5	2.787 (5)	O3···C22^{ii}	3.322 (7)
Ce1···C6	2.829 (5)	O3···C21^{ii}	3.448 (6)
Ce1···C7	2.722 (5)	O3···C18^{i}	3.586 (7)
Ce1···C8	2.742 (5)	C6···C23^{v}	3.568 (7)
Ce1···C9	2.857 (5)	C8···C22^{v}	3.536 (8)
Ce1···Cg1	2.5382 (3)	C8···C23^{v}	3.575 (8)
Ce1···Cg2	2.5439 (3)	C9···C22^{v}	3.407 (7)

F1···C19^{i}	3.571 (7)	C9···C23^{v}	3.520 (8)
F2···C12^{ii}	3.043 (7)	C10···C23^{v}	3.486 (7)
F2···C5^{iii}	3.271 (6)	C15···C27^{iv}	3.408 (8)
F2···C15^{iii}	3.369 (7)	C18···C18^{i}	3.57 (1)
F2···C4^{iii}	3.409 (6)	C23···Cg2^{vi}	3.340 (6)
O1—Ce1—N1	142.7 (1)	C16—C6—Cg2	172.4 (5)
O1—Ce1—N2	81.5 (1)	Ce1—C7—C6	79.3 (3)
O1—Ce1—C1	98.7 (1)	Ce1—C7—C8	75.6 (3)
O1—Ce1—C2	121.7 (1)	Ce1—C7—C17	109.6 (3)
O1—Ce1—C3	110.0 (1)	Ce1—C7—Cg2	68.6 (2)
O1—Ce1—C4	80.9 (1)	C6—C7—C8	107.5 (5)
O1—Ce1—C5	74.0 (1)	C6—C7—C17	126.1 (5)
O1—Ce1—C6	107.8 (1)	C6—C7—Cg2	53.9 (3)
O1—Ce1—C7	78.8 (1)	C8—C7—C17	126.3 (5)
O1—Ce1—C8	75.9 (1)	C8—C7—Cg2	53.7 (3)
O1—Ce1—C9	102.6 (1)	C17—C7—Cg2	178.2 (5)
O1—Ce1—Cg1	97.60 (8)	Ce1—C8—C7	74.1 (3)
O1—Ce1—Cg2	98.37 (7)	Ce1—C8—C9	79.9 (3)
N1—Ce1—N2	61.3 (1)	Ce1—C8—C18	116.5 (3)
N1—Ce1—C1	108.3 (1)	Ce1—C8—Cg2	67.8 (2)
N1—Ce1—C2	79.8 (2)	C7—C8—C9	108.3 (5)
N1—Ce1—C3	73.1 (2)	C7—C8—C18	127.4 (5)
N1—Ce1—C4	98.1 (1)	C7—C8—Cg2	54.0 (3)
N1—Ce1—C5	121.3 (1)	C9—C8—C18	124.1 (5)
N1—Ce1—C6	97.8 (1)	C9—C8—Cg2	54.2 (3)
N1—Ce1—C7	119.5 (1)	C18—C8—Cg2	175.6 (5)
N1—Ce1—C8	103.5 (2)	Ce1—C9—C8	70.9 (3)
N1—Ce1—C9	75.0 (1)	Ce1—C9—C10	78.4 (3)
N1—Ce1—Cg1	96.33 (9)	Ce1—C9—C19	120.3 (4)
N1—Ce1—Cg2	93.39 (9)	Ce1—C9—Cg2	62.8 (2)
N2—Ce1—C1	136.3 (1)	C8—C9—C10	107.3 (5)
N2—Ce1—C2	117.5 (2)	C8—C9—C19	126.5 (5)
N2—Ce1—C3	90.6 (1)	C8—C9—Cg2	53.9 (3)
N2—Ce1—C4	89.3 (2)	C10—C9—C19	126.0 (5)
N2—Ce1—C5	115.9 (2)	C10—C9—Cg2	53.4 (3)
N2—Ce1—C6	132.3 (1)	C19—C9—Cg2	176.9 (5)
N2—Ce1—C7	122.2 (2)	C6—C10—C9	109.0 (5)
N2—Ce1—C8	92.2 (2)	C6—C10—C20	125.1 (5)
N2—Ce1—C9	84.7 (1)	C6—C10—Cg2	54.7 (3)
N2—Ce1—Cg1	111.10 (10)	C9—C10—C20	124.2 (5)
N2—Ce1—Cg2	108.57 (10)	C9—C10—Cg2	54.4 (3)
C1—Ce1—C2	28.7 (2)	C20—C10—Cg2	167.6 (5)
C1—Ce1—C3	48.0 (2)	N1—C21—C22	123.6 (5)
C1—Ce1—C4	48.3 (2)	C21—C22—C23	119.2 (5)
C1—Ce1—C5	29.2 (1)	C22—C23—C24	118.7 (5)
C1—Ce1—C6	89.6 (2)	C23—C24—C25	119.2 (5)
C1—Ce1—C7	100.3 (2)	N1—C25—C24	122.0 (5)
C1—Ce1—C8	130.5 (2)	N1—C25—C26	115.9 (5)

C1—Ce1—C9	136.3 (2)	C24—C25—C26	122.1 (5)
C1—Ce1—Cg1	25.2 (1)	N2—C26—C25	116.7 (5)
C1—Ce1—Cg2	114.5 (1)	N2—C26—C27	121.3 (5)
C2—Ce1—C3	29.0 (2)	C25—C26—C27	121.9 (5)
C2—Ce1—C4	48.0 (2)	C26—C27—C28	119.8 (5)
C2—Ce1—C5	47.8 (2)	C27—C28—C29	118.9 (6)
C2—Ce1—C6	97.5 (2)	C28—C29—C30	118.5 (5)
C2—Ce1—C7	119.2 (2)	N2—C30—C29	123.9 (5)
C2—Ce1—C8	146.2 (2)	S1—C31—F1	113.2 (4)
C2—Ce1—C9	131.9 (2)	S1—C31—F2	109.5 (4)
C2—Ce1—Cg1	24.9 (1)	S1—C31—F3	111.9 (4)
C2—Ce1—Cg2	121.4 (1)	F1—C31—F2	107.0 (5)
C3—Ce1—C4	29.3 (2)	F1—C31—F3	107.6 (5)
C3—Ce1—C5	48.3 (2)	F2—C31—F3	107.4 (5)
C3—Ce1—C6	126.0 (2)	Ce1—Cg1—C1	90.7 (3)
C3—Ce1—C7	147.2 (2)	Ce1—Cg1—C2	92.0 (2)
C3—Ce1—C8	173.8 (2)	Ce1—Cg1—C3	90.4 (3)
C3—Ce1—C9	145.9 (2)	Ce1—Cg1—C4	88.0 (3)
C3—Ce1—Cg1	25.4 (1)	Ce1—Cg1—C5	88.8 (2)
C3—Ce1—Cg2	147.9 (1)	C1—Cg1—C2	71.7 (4)
C4—Ce1—C5	29.6 (2)	C1—Cg1—C3	143.9 (4)
C4—Ce1—C6	137.8 (2)	C1—Cg1—C4	144.3 (4)
C4—Ce1—C7	138.8 (2)	C1—Cg1—C5	71.9 (4)
C4—Ce1—C8	156.2 (2)	C2—Cg1—C3	72.2 (4)
C4—Ce1—C9	172.4 (2)	C2—Cg1—C4	144.0 (4)
C4—Ce1—Cg1	25.7 (1)	C2—Cg1—C5	143.7 (4)
C4—Ce1—Cg2	161.9 (1)	C3—Cg1—C4	71.8 (4)
C5—Ce1—C6	111.5 (2)	C3—Cg1—C5	144.1 (4)
C5—Ce1—C7	109.7 (2)	C4—Cg1—C5	72.3 (4)
C5—Ce1—C8	134.3 (2)	Ce1—Cg2—C6	90.6 (2)
C5—Ce1—C9	157.7 (2)	Ce1—Cg2—C7	85.1 (2)
C5—Ce1—Cg1	25.6 (1)	Ce1—Cg2—C8	86.2 (2)
C5—Ce1—Cg2	132.7 (1)	Ce1—Cg2—C9	92.1 (2)
C6—Ce1—C7	29.7 (1)	Ce1—Cg2—C10	96.0 (2)
C6—Ce1—C8	48.8 (2)	C6—Cg2—C7	72.2 (4)
C6—Ce1—C9	47.7 (2)	C6—Cg2—C8	144.4 (4)
C6—Ce1—Cg1	113.6 (1)	C6—Cg2—C9	143.7 (4)
C6—Ce1—Cg2	25.3 (1)	C6—Cg2—C10	71.5 (4)
C7—Ce1—C8	30.3 (2)	C7—Cg2—C8	72.3 (4)
C7—Ce1—C9	48.7 (2)	C7—Cg2—C9	144.2 (4)
C7—Ce1—Cg1	125.0 (1)	C7—Cg2—C10	143.7 (4)
C7—Ce1—Cg2	26.3 (1)	C8—Cg2—C9	71.9 (4)
C8—Ce1—C9	29.3 (2)	C8—Cg2—C10	144.0 (4)
C8—Ce1—Cg1	154.8 (1)	C9—Cg2—C10	72.2 (4)
C8—Ce1—Cg2	26.0 (1)	C1—C11—H11A	109.872
C9—Ce1—Cg1	156.1 (1)	C1—C11—H11B	109.542
C9—Ce1—Cg2	25.1 (1)	C1—C11—H11C	109.207
Cg1—Ce1—Cg2	138.91 (1)	H11A—C11—H11B	109.795
O1—S1—O2	114.4 (2)	H11A—C11—H11C	109.368

O1—S1—O3	113.9 (2)	H11B—C11—H11C	109.039
O1—S1—C31	104.5 (2)	C2—C12—H12A	109.352
O2—S1—O3	116.5 (2)	C2—C12—H12B	109.437
O2—S1—C31	101.9 (2)	C2—C12—H12C	109.500
O3—S1—C31	103.2 (3)	H12A—C12—H12B	109.346
Ce1—O1—S1	165.6 (2)	H12A—C12—H12C	109.595
Ce1—N1—C21	118.1 (3)	H12B—C12—H12C	109.598
Ce1—N1—C25	124.3 (3)	C3—C13—H13A	109.386
C21—N1—C25	117.3 (5)	C3—C13—H13B	109.372
Ce1—N2—C26	121.2 (3)	C3—C13—H13C	109.645
Ce1—N2—C30	121.1 (4)	H13A—C13—H13B	109.319
C26—N2—C30	117.5 (5)	H13A—C13—H13C	109.531
Ce1—C1—C2	76.4 (3)	H13B—C13—H13C	109.574
Ce1—C1—C5	74.0 (3)	C4—C14—H14A	109.234
Ce1—C1—C11	124.5 (4)	C4—C14—H14B	109.436
Ce1—C1—Cg1	64.0 (2)	C4—C14—H14C	109.214
C2—C1—C5	107.9 (5)	H14A—C14—H14B	109.789
C2—C1—C11	126.9 (5)	H14A—C14—H14C	109.399
C2—C1—Cg1	53.9 (3)	H14B—C14—H14C	109.753
C5—C1—C11	124.2 (5)	C5—C15—H15A	109.323
C5—C1—Cg1	54.0 (3)	C5—C15—H15B	109.200
C11—C1—Cg1	171.3 (5)	C5—C15—H15C	109.552
Ce1—C2—C1	74.8 (3)	H15A—C15—H15B	109.240
Ce1—C2—C3	74.5 (3)	H15A—C15—H15C	109.960
Ce1—C2—C12	124.8 (4)	H15B—C15—H15C	109.550
Ce1—C2—Cg1	63.2 (2)	C6—C16—H16A	109.465
C1—C2—C3	108.6 (5)	C6—C16—H16B	109.353
C1—C2—C12	124.1 (5)	C6—C16—H16C	109.337
C1—C2—Cg1	54.4 (3)	H16A—C16—H16B	109.548
C3—C2—C12	126.5 (6)	H16A—C16—H16C	109.760
C3—C2—Cg1	54.3 (3)	H16B—C16—H16C	109.363
C12—C2—Cg1	172.0 (5)	C7—C17—H17A	109.281
Ce1—C3—C2	76.5 (3)	C7—C17—H17B	109.130
Ce1—C3—C4	73.5 (3)	C7—C17—H17C	109.451
Ce1—C3—C13	121.1 (4)	H17A—C17—H17B	109.368
Ce1—C3—Cg1	64.2 (2)	H17A—C17—H17C	109.853
C2—C3—C4	107.5 (5)	H17B—C17—H17C	109.742
C2—C3—C13	128.2 (5)	C8—C18—H18A	109.155
C2—C3—Cg1	53.5 (3)	C8—C18—H18B	109.271
C4—C3—C13	124.0 (5)	C8—C18—H18C	109.329
C4—C3—Cg1	53.9 (3)	H18A—C18—H18B	109.655
C13—C3—Cg1	174.2 (5)	H18A—C18—H18C	109.809
Ce1—C4—C3	77.2 (3)	H18B—C18—H18C	109.606
Ce1—C4—C5	75.8 (3)	C9—C19—H19A	111.199
Ce1—C4—C14	115.9 (4)	C9—C19—H19B	111.115
Ce1—C4—Cg1	66.3 (2)	C9—C19—H19C	110.863
C3—C4—C5	108.1 (5)	H19A—C19—H19B	108.049
C3—C4—C14	126.5 (5)	H19A—C19—H19C	107.839
C3—C4—Cg1	54.3 (3)	H19B—C19—H19C	107.624

C5—C4—C14	125.3 (5)	C10—C20—H20A	109.283
C5—C4—Cg1	53.9 (3)	C10—C20—H20B	109.410
C14—C4—Cg1	177.6 (5)	C10—C20—H20C	109.368
Ce1—C5—C1	76.8 (3)	H20A—C20—H20B	109.620
Ce1—C5—C4	74.6 (3)	H20A—C20—H20C	109.491
Ce1—C5—C15	121.7 (4)	H20B—C20—H20C	109.654
Ce1—C5—Cg1	65.6 (2)	N1—C21—H21	118.305
C1—C5—C4	107.8 (5)	C22—C21—H21	118.050
C1—C5—C15	123.5 (5)	C21—C22—H22	120.035
C1—C5—Cg1	54.0 (3)	C23—C22—H22	120.806
C4—C5—C15	128.0 (5)	C22—C23—H23	120.432
C4—C5—Cg1	53.8 (3)	C24—C23—H23	120.873
C15—C5—Cg1	172.4 (5)	C23—C24—H24	120.197
Ce1—C6—C7	71.0 (3)	C25—C24—H24	120.591
Ce1—C6—C10	79.6 (3)	C26—C27—H27	119.979
Ce1—C6—C16	123.5 (3)	C28—C27—H27	120.231
Ce1—C6—Cg2	64.1 (2)	C27—C28—H28	120.632
C7—C6—C10	107.8 (5)	C29—C28—H28	120.450
C7—C6—C16	126.5 (5)	C28—C29—H29	121.253
C7—C6—Cg2	54.0 (3)	C30—C29—H29	120.212
C10—C6—C16	124.9 (5)	N2—C30—H30	117.967
C10—C6—Cg2	53.8 (3)	C29—C30—H30	118.178
Ce1—O1—S1—O2	74.3 (9)	C2i—Cg1i—C4i—C14i	110 (13)
Ce1—O1—S1—O3	−63.2 (9)	C2i—Cg1i—C5i—C4i	180.0 (5)
Ce1—O1—S1—C31	−175.1 (8)	C2i—Cg1i—C5i—C15i	−73 (4)
Ce1—N1—C21—C22	172.6 (4)	C3i—Ce1i—N1i—C21i	−78.8 (4)
Ce1—N1—C25—C24	−172.0 (4)	C3i—Ce1i—N1i—C25i	94.6 (4)
Ce1—N1—C25—C26	9.6 (6)	C3i—Ce1i—N2i—C26i	−69.6 (4)
Ce1—N2—C26—C25	3.4 (6)	C3i—Ce1i—N2i—C30i	115.4 (4)
Ce1—N2—C26—C27	−176.4 (4)	C3i—Ce1i—C1i—C5i	−77.2 (3)
Ce1—N2—C30—C29	175.6 (5)	C3i—Ce1i—C1i—C11i	162.0 (5)
Ce1—C1—C2—C3	−67.5 (4)	C3i—Ce1i—C1i—Cg1i	−19.9 (2)
Ce1—C1—C2—C12	122.0 (5)	C3i—Ce1i—C2i—C12i	124.0 (7)
Ce1—C1—C2—Cg1	−67.6 (2)	C3i—Ce1i—C2i—Cg1i	−57.4 (3)
Ce1—C1—C5—C4	68.8 (4)	C3i—Ce1i—C4i—C5i	112.7 (5)
Ce1—C1—C5—C15	−119.5 (5)	C3i—Ce1i—C4i—C14i	−124.6 (6)
Ce1—C1—C5—Cg1	69.2 (2)	C3i—Ce1i—C4i—Cg1i	56.3 (3)
Ce1—C1—Cg1—C2	91.8 (3)	C3i—Ce1i—C5i—C4i	−37.2 (3)
Ce1—C1—Cg1—C3	91.7 (6)	C3i—Ce1i—C5i—C15i	−162.7 (5)
Ce1—C1—Cg1—C4	−87.6 (6)	C3i—Ce1i—C5i—Cg1i	19.6 (2)
Ce1—C1—Cg1—C5	−88.5 (3)	C3i—Ce1i—C6i—C7i	−145.6 (3)
Ce1—C2—C1—C5	67.9 (4)	C3i—Ce1i—C6i—C10i	101.4 (3)
Ce1—C2—C1—C11	−123.1 (6)	C3i—Ce1i—C6i—C16i	−23.8 (5)
Ce1—C2—C1—Cg1	67.6 (2)	C3i—Ce1i—C6i—Cg2i	156.1 (2)
Ce1—C2—C3—C4	−67.5 (4)	C3i—Ce1i—C7i—C6i	57.8 (5)
Ce1—C2—C3—C13	119.1 (6)	C3i—Ce1i—C7i—C8i	169.2 (3)
Ce1—C2—C3—Cg1	−67.8 (2)	C3i—Ce1i—C7i—C17i	−67.0 (5)
Ce1—C2—Cg1—C1	−90.1 (3)	C3i—Ce1i—C7i—Cg2i	113.0 (3)
Ce1—C2—Cg1—C3	89.8 (3)	C3i—Ce1i—C8i—Cg2i	−13 (1)

Ce1—C2—Cg1—C4	89.3 (5)	C3i—Ce1i—C9i—C8i	−172.7 (3)
Ce1—C2—Cg1—C5	−90.7 (5)	C3i—Ce1i—C9i—C10i	−59.5 (4)
Ce1—C3—C2—C1	67.7 (4)	C3i—Ce1i—C9i—C19i	65.6 (5)
Ce1—C3—C2—C12	−122.1 (5)	C3i—Ce1i—C9i—Cg2i	−114.2 (3)
Ce1—C3—C2—Cg1	67.8 (2)	C3i—Ce1i—Cg1i—C4i	−71.8 (4)
Ce1—C3—C4—C5	−70.2 (4)	C3i—Ce1i—Cg1i—C5i	−144.1 (4)
Ce1—C3—C4—C14	113.0 (6)	C3i—Ce1i—Cg2i—C6i	−38.2 (3)
Ce1—C3—C4—Cg1	−69.8 (2)	C3i—Ce1i—Cg2i—C7i	−110.2 (3)
Ce1—C3—Cg1—C1	−91.8 (6)	C3i—Ce1i—Cg2i—C8i	177.2 (3)
Ce1—C3—Cg1—C2	−91.9 (3)	C3i—Ce1i—Cg2i—C9i	105.6 (3)
Ce1—C3—Cg1—C4	87.8 (3)	C3i—Ce1i—Cg2i—C10i	33.3 (3)
Ce1—C3—Cg1—C5	88.5 (6)	C3i—C2i—Ce1i—C4i	37.3 (3)
Ce1—C4—C3—C2	69.6 (4)	C3i—C2i—Ce1i—C5i	77.6 (3)
Ce1—C4—C3—C13	−116.7 (6)	C3i—C2i—Ce1i—C6i	−170.1 (3)
Ce1—C4—C3—Cg1	69.8 (2)	C3i—C2i—Ce1i—C7i	168.3 (3)
Ce1—C4—C5—C1	−70.3 (4)	C3i—C2i—Ce1i—C8i	−172.5 (3)
Ce1—C4—C5—C15	118.5 (6)	C3i—C2i—Ce1i—C9i	−132.6 (3)
Ce1—C4—C5—Cg1	−70.8 (2)	C3i—C2i—Ce1i—Cg1i	57.4 (3)
Ce1—C4—Cg1—C1	88.5 (6)	C3i—C2i—Ce1i—Cg2i	−161.2 (3)
Ce1—C4—Cg1—C2	−90.6 (5)	C3i—C2i—C1i—C5i	0.4 (6)
Ce1—C4—Cg1—C3	−91.1 (3)	C3i—C2i—C1i—C11i	169.4 (5)
Ce1—C4—Cg1—C5	89.4 (3)	C3i—C2i—C1i—Cg1i	0.1 (4)
Ce1—C5—C1—C2	−69.5 (4)	C3i—C2i—Cg1i—C4i	−0.5 (7)
Ce1—C5—C1—C11	121.1 (5)	C3i—C2i—Cg1i—C5i	179.6 (6)
Ce1—C5—C1—Cg1	−69.2 (2)	C3i—C4i—Ce1i—C5i	−112.7 (5)
Ce1—C5—C4—C3	71.2 (4)	C3i—C4i—Ce1i—C6i	−79.7 (4)
Ce1—C5—C4—C14	−112.0 (5)	C3i—C4i—Ce1i—C7i	−125.0 (3)
Ce1—C5—C4—Cg1	70.8 (2)	C3i—C4i—Ce1i—C8i	−173.7 (4)
Ce1—C5—Cg1—C1	91.2 (3)	C3i—C4i—Ce1i—Cg1i	−56.3 (3)
Ce1—C5—Cg1—C2	91.7 (5)	C3i—C4i—Ce1i—Cg2i	−97.0 (5)
Ce1—C5—Cg1—C3	−89.0 (6)	C3i—C4i—C5i—C15i	−170.4 (5)
Ce1—C5—Cg1—C4	−88.3 (3)	C3i—C4i—C5i—Cg1i	0.4 (4)
Ce1—C6—C7—C8	−71.1 (3)	C3i—C4i—Cg1i—C5i	−179.5 (4)
Ce1—C6—C7—C17	106.5 (5)	C3i—Cg1i—Ce1i—C4i	71.8 (4)
Ce1—C6—C7—Cg2	−71.2 (2)	C3i—Cg1i—Ce1i—C5i	144.1 (4)
Ce1—C6—C10—C9	64.4 (4)	C3i—Cg1i—Ce1i—C6i	−125.1 (3)
Ce1—C6—C10—C20	−129.8 (5)	C3i—Cg1i—Ce1i—C7i	−156.7 (3)
Ce1—C6—C10—Cg2	65.4 (2)	C3i—Cg1i—Ce1i—C8i	−165.5 (4)
Ce1—C6—Cg2—C7	84.6 (3)	C3i—Cg1i—Ce1i—C9i	−90.6 (4)
Ce1—C6—Cg2—C8	84.3 (5)	C3i—Cg1i—Ce1i—Cg2i	−126.2 (3)
Ce1—C6—Cg2—C9	−94.4 (5)	C3i—Cg1i—C1i—C5i	−179.8 (6)
Ce1—C6—Cg2—C10	−96.2 (3)	C3i—Cg1i—C1i—C11i	−98 (3)
Ce1—C7—C6—C10	71.9 (4)	C3i—Cg1i—C2i—C12i	−98 (4)
Ce1—C7—C6—C16	−118.2 (5)	C3i—Cg1i—C4i—C5i	179.5 (4)
Ce1—C7—C6—Cg2	71.2 (2)	C3i—Cg1i—C4i—C14i	109 (13)
Ce1—C7—C8—C9	−73.3 (4)	C3i—Cg1i—C5i—C4i	−0.7 (7)
Ce1—C7—C8—C18	111.4 (5)	C3i—Cg1i—C5i—C15i	105 (3)
Ce1—C7—C8—Cg2	−73.8 (2)	C4i—Ce1i—N1i—C21i	−94.4 (4)
Ce1—C7—Cg2—C6	−92.2 (3)	C4i—Ce1i—N1i—C25i	79.1 (4)

Ce1—C7—Cg2—C8	87.6 (3)	C4i—Ce1i—N2i—C26i	−98.8 (4)
Ce1—C7—Cg2—C9	86.7 (5)	C4i—Ce1i—N2i—C30i	86.1 (5)
Ce1—C7—Cg2—C10	−93.5 (5)	C4i—Ce1i—C1i—C5i	−37.5 (3)
Ce1—C8—C7—C6	73.6 (4)	C4i—Ce1i—C1i—C11i	−158.3 (5)
Ce1—C8—C7—C17	−104.0 (5)	C4i—Ce1i—C1i—Cg1i	19.8 (2)
Ce1—C8—C7—Cg2	73.8 (2)	C4i—Ce1i—C2i—C12i	161.2 (6)
Ce1—C8—C9—C10	−70.7 (4)	C4i—Ce1i—C2i—Cg1i	−20.1 (2)
Ce1—C8—C9—C19	114.0 (5)	C4i—Ce1i—C3i—C13i	120.2 (6)
Ce1—C8—C9—Cg2	−69.8 (2)	C4i—Ce1i—C3i—Cg1i	−57.4 (3)
Ce1—C8—Cg2—C6	−85.7 (5)	C4i—Ce1i—C5i—C15i	−125.5 (6)
Ce1—C8—Cg2—C7	−86.0 (3)	C4i—Ce1i—C5i—Cg1i	56.8 (3)
Ce1—C8—Cg2—C9	93.4 (3)	C4i—Ce1i—C6i—C7i	−109.1 (4)
Ce1—C8—Cg2—C10	95.1 (5)	C4i—Ce1i—C6i—C10i	137.9 (3)
Ce1—C9—C8—C7	69.4 (3)	C4i—Ce1i—C6i—C16i	12.7 (6)
Ce1—C9—C8—C18	−115.2 (5)	C4i—Ce1i—C6i—Cg2i	−167.5 (2)
Ce1—C9—C8—Cg2	69.8 (2)	C4i—Ce1i—C7i—C6i	105.6 (4)
Ce1—C9—C10—C6	−63.7 (4)	C4i—Ce1i—C7i—C8i	−143.0 (3)
Ce1—C9—C10—C20	130.4 (5)	C4i—Ce1i—C7i—C17i	−19.2 (5)
Ce1—C9—C10—Cg2	−64.7 (2)	C4i—Ce1i—C7i—Cg2i	160.8 (2)
Ce1—C9—Cg2—C6	93.9 (5)	C4i—Ce1i—C8i—C7i	79.2 (5)
Ce1—C9—Cg2—C7	−84.5 (5)	C4i—Ce1i—C8i—C9i	−168.3 (4)
Ce1—C9—Cg2—C8	−85.3 (3)	C4i—Ce1i—C8i—C18i	−45.1 (7)
Ce1—C9—Cg2—C10	95.7 (3)	C4i—Ce1i—C8i—Cg2i	136.3 (3)
Ce1—Cg1—C1—C2	−91.8 (3)	C4i—Ce1i—C9i—Cg2i	−159 (1)
Ce1—Cg1—C1—C5	88.5 (3)	C4i—Ce1i—Cg1i—C5i	−72.3 (4)
Ce1—Cg1—C1—C11	169 (3)	C4i—Ce1i—Cg2i—C6i	27.9 (5)
Ce1—Cg1—C2—C1	90.1 (3)	C4i—Ce1i—Cg2i—C7i	−44.1 (5)
Ce1—Cg1—C2—C3	−89.8 (3)	C4i—Ce1i—Cg2i—C8i	−116.6 (5)
Ce1—Cg1—C2—C12	172 (4)	C4i—Ce1i—Cg2i—C9i	171.7 (4)
Ce1—Cg1—C3—C2	91.9 (3)	C4i—Ce1i—Cg2i—C10i	99.4 (5)
Ce1—Cg1—C3—C4	−87.8 (3)	C4i—C3i—Ce1i—C5i	37.6 (3)
Ce1—Cg1—C3—C13	−158 (5)	C4i—C3i—Ce1i—C6i	125.3 (3)
Ce1—Cg1—C4—C3	91.1 (3)	C4i—C3i—Ce1i—C7i	94.1 (4)
Ce1—Cg1—C4—C5	−89.4 (3)	C4i—C3i—Ce1i—C9i	−168.9 (3)
Ce1—Cg1—C4—C14	−159 (13)	C4i—C3i—Ce1i—Cg1i	57.4 (3)
Ce1—Cg1—C5—C1	−91.2 (3)	C4i—C3i—Ce1i—Cg2i	144.4 (3)
Ce1—Cg1—C5—C4	88.3 (3)	C4i—C3i—C2i—C12i	170.4 (5)
Ce1—Cg1—C5—C15	−165 (3)	C4i—C3i—C2i—Cg1i	0.3 (3)
Ce1—Cg2—C6—C7	−84.6 (3)	C4i—C3i—Cg1i—C5i	0.7 (7)
Ce1—Cg2—C6—C10	96.2 (3)	C4i—C5i—Ce1i—C6i	−156.8 (3)
Ce1—Cg2—C6—C16	178 (3)	C4i—C5i—Ce1i—C7i	171.5 (3)
Ce1—Cg2—C7—C6	92.2 (3)	C4i—C5i—Ce1i—C8i	150.5 (3)
Ce1—Cg2—C7—C8	−87.6 (3)	C4i—C5i—Ce1i—C9i	−175.8 (4)
Ce1—Cg2—C7—C17	2(16)	C4i—C5i—Ce1i—Cg1i	−56.8 (3)
Ce1—Cg2—C8—C7	86.0 (3)	C4i—C5i—Ce1i—Cg2i	−173.4 (3)
Ce1—Cg2—C8—C9	−93.4 (3)	C4i—C5i—C1i—C11i	−170.1 (5)
Ce1—Cg2—C8—C18	−163 (7)	C4i—C5i—C1i—Cg1i	−0.5 (4)
Ce1—Cg2—C9—C8	85.3 (3)	C4i—Cg1i—Ce1i—C5i	72.3 (4)
Ce1—Cg2—C9—C10	−95.7 (3)	C4i—Cg1i—Ce1i—C6i	163.1 (3)

Ce1—Cg2—C9—C19	−176 (9)	C4i—Cg1i—Ce1i—C7i	131.5 (3)
Ce1—Cg2—C10—C6	−88.6 (3)	C4i—Cg1i—Ce1i—C8i	122.7 (4)
Ce1—Cg2—C10—C9	90.3 (3)	C4i—Cg1i—Ce1i—C9i	−162.4 (4)
Ce1—Cg2—C10—C20	178 (2)	C4i—Cg1i—Ce1i—Cg2i	162.0 (3)
S1—O1—Ce1—N1	41.3 (10)	C4i—Cg1i—C1i—C5i	0.9 (7)
S1—O1—Ce1—N2	40.6 (9)	C4i—Cg1i—C1i—C11i	81 (3)
S1—O1—Ce1—C1	−95.2 (9)	C4i—Cg1i—C2i—C12i	−98 (4)
S1—O1—Ce1—C2	−76.5 (9)	C4i—Cg1i—C3i—C13i	−70 (5)
S1—O1—Ce1—C3	−46.8 (9)	C4i—Cg1i—C5i—C15i	106 (4)
S1—O1—Ce1—C4	−50.1 (9)	C5i—Ce1i—N1i—C21i	−74.6 (4)
S1—O1—Ce1—C5	−79.6 (9)	C5i—Ce1i—N1i—C25i	98.8 (4)
S1—O1—Ce1—C6	172.5 (9)	C5i—Ce1i—N2i—C26i	−112.3 (4)
S1—O1—Ce1—C7	166.0 (9)	C5i—Ce1i—N2i—C30i	72.7 (5)
S1—O1—Ce1—C8	135.1 (9)	C5i—Ce1i—C1i—C11i	−120.8 (6)
S1—O1—Ce1—C9	123.2 (9)	C5i—Ce1i—C1i—Cg1i	57.3 (3)
S1—O1—Ce1—Cg1	−69.7 (9)	C5i—Ce1i—C2i—C12i	−158.5 (6)
S1—O1—Ce1—Cg2	148.3 (9)	C5i—Ce1i—C2i—Cg1i	20.2 (2)
F1—C31—S1—O1	65.7 (4)	C5i—Ce1i—C3i—C13i	157.8 (5)
F1—C31—S1—O2	−174.9 (4)	C5i—Ce1i—C3i—Cg1i	−19.8 (2)
F1—C31—S1—O3	−53.7 (4)	C5i—Ce1i—C4i—C14i	122.6 (6)
F2—C31—S1—O1	−175.0 (4)	C5i—Ce1i—C4i—Cg1i	−56.4 (3)
F2—C31—S1—O2	−55.6 (4)	C5i—Ce1i—C6i—C7i	−92.2 (3)
F2—C31—S1—O3	65.6 (4)	C5i—Ce1i—C6i—C10i	154.7 (3)
F3—C31—S1—O1	−56.1 (4)	C5i—Ce1i—C6i—C16i	29.6 (5)
F3—C31—S1—O2	63.3 (4)	C5i—Ce1i—C6i—Cg2i	−150.6 (2)
F3—C31—S1—O3	−175.5 (4)	C5i—Ce1i—C7i—C6i	99.2 (3)
O1—Ce1—N1—C21	−179.9 (3)	C5i—Ce1i—C7i—C8i	−149.4 (3)
O1—Ce1—N1—C25	−6.4 (5)	C5i—Ce1i—C7i—C17i	−25.5 (4)
O1—Ce1—N2—C26	−179.8 (4)	C5i—Ce1i—C7i—Cg2i	154.4 (2)
O1—Ce1—N2—C30	5.2 (4)	C5i—Ce1i—C8i—C7i	42.1 (4)
O1—Ce1—C1—C2	145.5 (3)	C5i—Ce1i—C8i—C9i	154.5 (3)
O1—Ce1—C1—C5	32.0 (3)	C5i—Ce1i—C8i—C18i	−82.2 (5)
O1—Ce1—C1—C11	−88.8 (5)	C5i—Ce1i—C8i—Cg2i	99.2 (3)
O1—Ce1—C1—Cg1	89.3 (2)	C5i—Ce1i—C9i—C8i	−54.2 (5)
O1—Ce1—C2—C1	−41.1 (4)	C5i—Ce1i—C9i—C10i	58.9 (6)
O1—Ce1—C2—C3	73.6 (4)	C5i—Ce1i—C9i—C19i	−176.0 (4)
O1—Ce1—C2—C12	−162.5 (5)	C5i—Ce1i—C9i—Cg2i	4.2 (6)
O1—Ce1—C2—Cg1	16.2 (4)	C5i—Ce1i—Cg2i—C6i	38.4 (3)
O1—Ce1—C3—C2	−119.6 (3)	C5i—Ce1i—Cg2i—C7i	−33.6 (3)
O1—Ce1—C3—C4	−6.5 (4)	C5i—Ce1i—Cg2i—C8i	−106.1 (3)
O1—Ce1—C3—C13	113.7 (4)	C5i—Ce1i—Cg2i—C9i	−177.8 (3)
O1—Ce1—C3—Cg1	−63.9 (3)	C5i—Ce1i—Cg2i—C10i	109.9 (3)
O1—Ce1—C4—C3	173.8 (4)	C5i—C1i—Ce1i—C6i	139.9 (3)
O1—Ce1—C4—C5	−73.4 (3)	C5i—C1i—Ce1i—C7i	112.1 (3)
O1—Ce1—C4—C14	49.2 (4)	C5i—C1i—Ce1i—C8i	110.8 (3)
O1—Ce1—C4—Cg1	−129.8 (3)	C5i—C1i—Ce1i—C9i	150.8 (3)
O1—Ce1—C5—C1	−147.0 (3)	C5i—C1i—Ce1i—Cg1i	−57.3 (3)
O1—Ce1—C5—C4	100.0 (3)	C5i—C1i—Ce1i—Cg2i	135.4 (3)
O1—Ce1—C5—C15	−25.5 (4)	C5i—C1i—C2i—C12i	−170.1 (5)

O1—Ce1—C5—Cg1	156.8 (3)	C5i—C1i—C2i—Cg1i	0.3 (3)
O1—Ce1—C6—C7	−12.9 (3)	C5i—C4i—Ce1i—C6i	33.1 (4)
O1—Ce1—C6—C10	−126.0 (3)	C5i—C4i—Ce1i—C7i	−12.2 (4)
O1—Ce1—C6—C16	108.9 (4)	C5i—C4i—Ce1i—C8i	−61.0 (6)
O1—Ce1—C6—Cg2	−71.3 (3)	C5i—C4i—Ce1i—Cg1i	56.4 (3)
O1—Ce1—C7—C6	167.5 (3)	C5i—C4i—Ce1i—Cg2i	15.7 (6)
O1—Ce1—C7—C8	−81.1 (3)	C5i—C4i—C3i—C13i	173.0 (5)
O1—Ce1—C7—C17	42.7 (4)	C5i—C4i—C3i—Cg1i	−0.4 (4)
O1—Ce1—C7—Cg2	−137.3 (3)	C5i—Cg1i—Ce1i—C6i	90.8 (3)
O1—Ce1—C8—C7	91.9 (3)	C5i—Cg1i—Ce1i—C7i	59.1 (3)
O1—Ce1—C8—C9	−155.6 (3)	C5i—Cg1i—Ce1i—C8i	50.4 (4)
O1—Ce1—C8—C18	−32.4 (4)	C5i—Cg1i—Ce1i—C9i	125.2 (4)
O1—Ce1—C8—Cg2	149.0 (3)	C5i—Cg1i—Ce1i—Cg2i	89.7 (3)
O1—Ce1—C9—C8	24.2 (3)	C5i—Cg1i—C1i—C11i	81 (3)
O1—Ce1—C9—C10	137.4 (3)	C5i—Cg1i—C2i—C12i	81 (4)
O1—Ce1—C9—C19	−97.5 (4)	C5i—Cg1i—C3i—C13i	−70 (5)
O1—Ce1—C9—Cg2	82.7 (2)	C5i—Cg1i—C4i—C14i	−69 (13)
O1—Ce1—Cg1—C1	−94.4 (3)	C6i—Ce1i—N1i—C21i	46.5 (4)
O1—Ce1—Cg1—C2	−166.1 (3)	C6i—Ce1i—N1i—C25i	−140.1 (4)
O1—Ce1—Cg1—C3	121.7 (3)	C6i—Ce1i—N2i—C26i	73.9 (4)
O1—Ce1—Cg1—C4	49.9 (3)	C6i—Ce1i—N2i—C30i	−101.1 (5)
O1—Ce1—Cg1—C5	−22.5 (3)	C6i—Ce1i—C1i—C11i	19.1 (5)
O1—Ce1—Cg2—C6	114.3 (3)	C6i—Ce1i—C1i—Cg1i	−162.8 (3)
O1—Ce1—Cg2—C7	42.2 (3)	C6i—Ce1i—C2i—C12i	−46.1 (5)
O1—Ce1—Cg2—C8	−30.3 (3)	C6i—Ce1i—C2i—Cg1i	132.5 (3)
O1—Ce1—Cg2—C9	−102.0 (3)	C6i—Ce1i—C3i—C13i	−114.5 (5)
O1—Ce1—Cg2—C10	−174.3 (3)	C6i—Ce1i—C3i—Cg1i	67.9 (3)
N1—Ce1—N2—C26	0.7 (4)	C6i—Ce1i—C4i—C14i	155.7 (4)
N1—Ce1—N2—C30	−174.3 (5)	C6i—Ce1i—C4i—Cg1i	−23.3 (4)
N1—Ce1—C1—C2	−8.5 (3)	C6i—Ce1i—C5i—C15i	77.7 (4)
N1—Ce1—C1—C5	−122.0 (3)	C6i—Ce1i—C5i—Cg1i	−100.0 (3)
N1—Ce1—C1—C11	117.3 (5)	C6i—Ce1i—C7i—C8i	111.4 (5)
N1—Ce1—C1—Cg1	−64.7 (3)	C6i—Ce1i—C7i—C17i	−124.7 (5)
N1—Ce1—C2—C1	171.8 (3)	C6i—Ce1i—C7i—Cg2i	55.2 (3)
N1—Ce1—C2—C3	−73.4 (3)	C6i—Ce1i—C8i—C7i	−37.8 (3)
N1—Ce1—C2—C12	50.5 (5)	C6i—Ce1i—C8i—C9i	74.6 (3)
N1—Ce1—C2—Cg1	−130.8 (3)	C6i—Ce1i—C8i—C18i	−162.2 (5)
N1—Ce1—C3—C2	99.6 (3)	C6i—Ce1i—C8i—Cg2i	19.3 (2)
N1—Ce1—C3—C4	−147.2 (4)	C6i—Ce1i—C9i—C8i	−78.4 (3)
N1—Ce1—C3—C13	−27.1 (4)	C6i—Ce1i—C9i—C10i	34.7 (3)
N1—Ce1—C3—Cg1	155.4 (3)	C6i—Ce1i—C9i—C19i	159.8 (5)
N1—Ce1—C4—C3	31.5 (4)	C6i—Ce1i—C9i—Cg2i	−20.0 (2)
N1—Ce1—C4—C5	144.3 (3)	C6i—Ce1i—Cg2i—C7i	−72.0 (4)
N1—Ce1—C4—C14	−93.1 (4)	C6i—Ce1i—Cg2i—C8i	−144.5 (4)
N1—Ce1—C4—Cg1	87.9 (3)	C6i—Ce1i—Cg2i—C9i	143.8 (4)
N1—Ce1—C5—C1	70.4 (4)	C6i—Ce1i—Cg2i—C10i	71.5 (4)
N1—Ce1—C5—C4	−42.6 (4)	C6i—C7i—Ce1i—C8i	−111.4 (5)
N1—Ce1—C5—C15	−168.0 (4)	C6i—C7i—Ce1i—C9i	−74.5 (3)
N1—Ce1—C5—Cg1	14.2 (3)	C6i—C7i—Ce1i—Cg1i	76.0 (3)

N1—Ce1—C6—C7	139.7 (3)	C6i—C7i—Ce1i—Cg2i	−55.2 (3)
N1—Ce1—C6—C10	26.6 (3)	C6i—C7i—C8i—C9i	0.3 (6)
N1—Ce1—C6—C16	−98.6 (4)	C6i—C7i—C8i—C18i	−174.9 (5)
N1—Ce1—C6—Cg2	81.3 (3)	C6i—C7i—C8i—Cg2i	−0.2 (3)
N1—Ce1—C7—C6	−47.5 (4)	C6i—C7i—Cg2i—C8i	179.8 (4)
N1—Ce1—C7—C8	64.0 (3)	C6i—C7i—Cg2i—C9i	179.0 (5)
N1—Ce1—C7—C17	−172.2 (3)	C6i—C7i—Cg2i—C10i	−1.3 (6)
N1—Ce1—C7—Cg2	7.7 (3)	C6i—C10i—C9i—C8i	1.8 (6)
N1—Ce1—C8—C7	−126.5 (3)	C6i—C10i—C9i—C19i	177.2 (5)
N1—Ce1—C8—C9	−14.0 (3)	C6i—C10i—C9i—Cg2i	1.0 (3)
N1—Ce1—C8—C18	109.2 (4)	C6i—C10i—Cg2i—C7i	1.3 (6)
N1—Ce1—C8—Cg2	−69.4 (3)	C6i—C10i—Cg2i—C8i	179.5 (5)
N1—Ce1—C9—C8	165.9 (3)	C6i—C10i—Cg2i—C9i	−178.9 (4)
N1—Ce1—C9—C10	−81.0 (3)	C6i—Cg2i—Ce1i—C7i	72.0 (4)
N1—Ce1—C9—C19	44.1 (4)	C6i—Cg2i—Ce1i—C8i	144.5 (4)
N1—Ce1—C9—Cg2	−135.7 (3)	C6i—Cg2i—Ce1i—C9i	−143.8 (4)
N1—Ce1—Cg1—C1	120.3 (3)	C6i—Cg2i—Ce1i—Cg1i	2.4 (3)
N1—Ce1—Cg1—C2	48.6 (3)	C6i—Cg2i—C7i—C8i	−179.8 (4)
N1—Ce1—Cg1—C3	−23.6 (3)	C6i—Cg2i—C7i—C17i	−90 (16)
N1—Ce1—Cg1—C4	−95.4 (3)	C6i—Cg2i—C8i—C7i	0.3 (6)
N1—Ce1—Cg1—C5	−167.8 (3)	C6i—Cg2i—C8i—C9i	−179.2 (5)
N1i—Ce1i—Cg2i—C6i	−101.2 (3)	C6i—Cg2i—C8i—C18i	110 (7)
N1i—Ce1i—Cg2i—C7i	−173.3 (3)	C6i—Cg2i—C9i—C8i	179.2 (5)
N1i—Ce1i—Cg2i—C8i	114.2 (3)	C6i—Cg2i—C9i—C10i	−1.8 (6)
N1i—Ce1i—Cg2i—C9i	42.5 (3)	C6i—Cg2i—C9i—C19i	−82 (9)
N1i—Ce1i—Cg2i—C10i	−29.7 (3)	C6i—Cg2i—C10i—C9i	178.9 (4)
N1i—C21i—C22i—C23i	−0.3 (9)	C6i—Cg2i—C10i—C20i	−93 (2)
N1i—C25i—C24i—C23i	−0.2 (9)	C7i—Ce1i—N1i—C21i	68.1 (4)
N1i—C25i—C26i—N2i	−8.2 (7)	C7i—Ce1i—N1i—C25i	−118.4 (4)
N1i—C25i—C26i—C27i	171.7 (5)	C7i—Ce1i—N2i—C26i	109.3 (4)
N2i—Ce1i—N1i—C21i	−179.1 (4)	C7i—Ce1i—N2i—C30i	−65.7 (5)
N2i—Ce1i—N1i—C25i	−5.7 (4)	C7i—Ce1i—C1i—C11i	−8.7 (5)
N2i—Ce1i—C1i—C2i	58.7 (4)	C7i—Ce1i—C1i—Cg1i	169.4 (2)
N2i—Ce1i—C1i—C5i	−54.8 (4)	C7i—Ce1i—C2i—C12i	−67.7 (6)
N2i—Ce1i—C1i—C11i	−175.5 (4)	C7i—Ce1i—C2i—Cg1i	111.0 (3)
N2i—Ce1i—C1i—Cg1i	2.5 (4)	C7i—Ce1i—C3i—C13i	−145.7 (4)
N2i—Ce1i—C2i—C1i	−138.3 (3)	C7i—Ce1i—C3i—Cg1i	36.7 (4)
N2i—Ce1i—C2i—C3i	−23.5 (4)	C7i—Ce1i—C4i—C14i	110.4 (4)
N2i—Ce1i—C2i—C12i	100.4 (5)	C7i—Ce1i—C4i—Cg1i	−68.6 (4)
N2i—Ce1i—C2i—Cg1i	−80.9 (3)	C7i—Ce1i—C5i—C15i	46.0 (5)
N2i—Ce1i—C3i—C2i	159.2 (3)	C7i—Ce1i—C5i—Cg1i	−131.7 (2)
N2i—Ce1i—C3i—C4i	−87.6 (3)	C7i—Ce1i—C6i—C10i	−113.1 (5)
N2i—Ce1i—C3i—C13i	32.6 (5)	C7i—Ce1i—C6i—C16i	121.8 (6)
N2i—Ce1i—C3i—Cg1i	−145.0 (3)	C7i—Ce1i—C6i—Cg2i	−58.4 (3)
N2i—Ce1i—C4i—C3i	92.4 (3)	C7i—Ce1i—C8i—C9i	112.5 (5)
N2i—Ce1i—C4i—C5i	−154.9 (3)	C7i—Ce1i—C8i—C18i	−124.3 (6)
N2i—Ce1i—C4i—C14i	−32.2 (4)	C7i—Ce1i—C8i—Cg2i	57.1 (3)
N2i—Ce1i—C4i—Cg1i	148.7 (3)	C7i—Ce1i—C9i—C8i	−38.3 (3)
N2i—Ce1i—C5i—C1i	141.2 (3)	C7i—Ce1i—C9i—C10i	74.9 (3)

N2i—Ce1i—C5i—C4i	28.1 (4)	C7i—Ce1i—C9i—C19i	−160.0 (5)
N2i—Ce1i—C5i—C15i	−97.3 (4)	C7i—Ce1i—C9i—Cg2i	20.2 (2)
N2i—Ce1i—C5i—Cg1i	85.0 (3)	C7i—Ce1i—Cg2i—C8i	−72.5 (4)
N2i—Ce1i—C6i—C7i	81.7 (4)	C7i—Ce1i—Cg2i—C9i	−144.2 (4)
N2i—Ce1i—C6i—C10i	−31.3 (4)	C7i—Ce1i—Cg2i—C10i	143.5 (4)
N2i—Ce1i—C6i—C16i	−156.5 (4)	C7i—C6i—Ce1i—C8i	38.6 (3)
N2i—Ce1i—C6i—Cg2i	23.3 (3)	C7i—C6i—Ce1i—C9i	78.2 (3)
N2i—Ce1i—C7i—C6i	−120.2 (3)	C7i—C6i—Ce1i—Cg1i	−119.9 (3)
N2i—Ce1i—C7i—C8i	−8.8 (4)	C7i—C6i—Ce1i—Cg2i	58.4 (3)
N2i—Ce1i—C7i—C17i	115.1 (4)	C7i—C6i—C10i—C9i	−1.6 (6)
N2i—Ce1i—C7i—Cg2i	−65.0 (3)	C7i—C6i—C10i—C20i	164.2 (5)
N2i—Ce1i—C8i—C7i	172.6 (3)	C7i—C6i—C10i—Cg2i	−0.7 (3)
N2i—Ce1i—C8i—C9i	−75.0 (3)	C7i—C6i—Cg2i—C8i	−0.3 (6)
N2i—Ce1i—C8i—C18i	48.2 (4)	C7i—C6i—Cg2i—C9i	−179.0 (5)
N2i—Ce1i—C8i—Cg2i	−130.3 (3)	C7i—C6i—Cg2i—C10i	179.2 (4)
N2i—Ce1i—C9i—C8i	104.2 (3)	C7i—C8i—Ce1i—C9i	−112.5 (5)
N2i—Ce1i—C9i—C10i	−142.6 (3)	C7i—C8i—Ce1i—Cg1i	14.4 (5)
N2i—Ce1i—C9i—C19i	−17.5 (4)	C7i—C8i—Ce1i—Cg2i	−57.1 (3)
N2i—Ce1i—C9i—Cg2i	162.7 (3)	C7i—C8i—C9i—C10i	−1.3 (6)
N2i—Ce1i—Cg1i—C1i	−178.1 (3)	C7i—C8i—C9i—C19i	−176.6 (5)
N2i—Ce1i—Cg1i—C2i	110.1 (3)	C7i—C8i—C9i—Cg2i	−0.4 (3)
N2i—Ce1i—Cg1i—C3i	38.0 (3)	C7i—C8i—Cg2i—C9i	179.5 (4)
N2i—Ce1i—Cg1i—C4i	−33.8 (3)	C7i—C8i—Cg2i—C10i	−178.9 (5)
N2i—Ce1i—Cg1i—C5i	−106.2 (3)	C7i—Cg2i—Ce1i—C8i	72.5 (4)
N2i—Ce1i—Cg2i—C6i	−162.0 (3)	C7i—Cg2i—Ce1i—C9i	144.2 (4)
N2i—Ce1i—Cg2i—C7i	126.0 (3)	C7i—Cg2i—Ce1i—Cg1i	−69.6 (3)
N2i—Ce1i—Cg2i—C8i	53.5 (3)	C7i—Cg2i—C6i—C10i	−179.2 (4)
N2i—Ce1i—Cg2i—C9i	−18.2 (3)	C7i—Cg2i—C6i—C16i	−96 (4)
N2i—Ce1i—Cg2i—C10i	−90.5 (3)	C7i—Cg2i—C8i—C9i	−179.5 (4)
N2i—C26i—C25i—C24i	173.4 (5)	C7i—Cg2i—C8i—C18i	110 (7)
N2i—C26i—C27i—C28i	1.7 (9)	C7i—Cg2i—C9i—C8i	0.8 (6)
N2i—C30i—C29i—C28i	0(1)	C7i—Cg2i—C9i—C10i	179.8 (5)
C1i—Ce1i—N1i—C21i	−45.7 (4)	C7i—Cg2i—C9i—C19i	98 (9)
C1i—Ce1i—N1i—C25i	127.8 (4)	C7i—Cg2i—C10i—C9i	−179.8 (5)
C1i—Ce1i—N2i—C26i	−86.0 (4)	C7i—Cg2i—C10i—C20i	−91 (2)
C1i—Ce1i—N2i—C30i	98.9 (5)	C8i—Ce1i—N1i—C21i	95.8 (4)
C1i—Ce1i—C2i—C3i	114.7 (5)	C8i—Ce1i—N1i—C25i	−90.7 (4)
C1i—Ce1i—C2i—C12i	−121.3 (7)	C8i—Ce1i—N2i—C26i	104.9 (4)
C1i—Ce1i—C2i—Cg1i	57.4 (3)	C8i—Ce1i—N2i—C30i	−70.1 (5)
C1i—Ce1i—C3i—C2i	−36.0 (3)	C8i—Ce1i—C1i—C11i	−10.0 (5)
C1i—Ce1i—C3i—C4i	77.1 (4)	C8i—Ce1i—C1i—Cg1i	168.1 (2)
C1i—Ce1i—C3i—C13i	−162.7 (5)	C8i—Ce1i—C2i—C12i	−48.5 (6)
C1i—Ce1i—C3i—Cg1i	19.8 (2)	C8i—Ce1i—C2i—Cg1i	130.2 (3)
C1i—Ce1i—C4i—C3i	−75.8 (4)	C8i—Ce1i—C3i—Cg1i	98 (1)
C1i—Ce1i—C4i—C5i	36.9 (3)	C8i—Ce1i—C4i—C14i	61.7 (6)
C1i—Ce1i—C4i—C14i	159.6 (5)	C8i—Ce1i—C4i—Cg1i	−117.4 (4)
C1i—Ce1i—C4i—Cg1i	−19.5 (2)	C8i—Ce1i—C5i—C15i	25.0 (5)
C1i—Ce1i—C5i—C4i	−113.0 (5)	C8i—Ce1i—C5i—Cg1i	−152.7 (2)
C1i—Ce1i—C5i—C15i	121.5 (6)	C8i—Ce1i—C6i—C10i	−74.5 (3)

C1i—Ce1i—C5i—Cg1i	−56.2 (3)	C8i—Ce1i—C6i—C16i	160.4 (5)
C1i—Ce1i—C6i—C7i	−112.0 (3)	C8i—Ce1i—C6i—Cg2i	−19.8 (2)
C1i—Ce1i—C6i—C10i	135.0 (3)	C8i—Ce1i—C7i—C17i	123.9 (5)
C1i—Ce1i—C6i—C16i	9.8 (4)	C8i—Ce1i—C7i—Cg2i	−56.2 (3)
C1i—Ce1i—C6i—Cg2i	−170.3 (3)	C8i—Ce1i—C9i—C10i	113.1 (5)
C1i—Ce1i—C7i—C6i	70.5 (3)	C8i—Ce1i—C9i—C19i	−121.8 (6)
C1i—Ce1i—C7i—C8i	−178.1 (3)	C8i—Ce1i—C9i—Cg2i	58.5 (3)
C1i—Ce1i—C7i—C17i	−54.2 (4)	C8i—Ce1i—Cg2i—C9i	−71.7 (4)
C1i—Ce1i—C7i—Cg2i	125.7 (2)	C8i—Ce1i—Cg2i—C10i	−144.0 (4)
C1i—Ce1i—C8i—C7i	2.5 (4)	C8i—C7i—Ce1i—C9i	37.0 (3)
C1i—Ce1i—C8i—C9i	114.9 (3)	C8i—C7i—Ce1i—Cg1i	−172.6 (3)
C1i—Ce1i—C8i—C18i	−121.9 (4)	C8i—C7i—Ce1i—Cg2i	56.2 (3)
C1i—Ce1i—C8i—Cg2i	59.6 (3)	C8i—C7i—C6i—C10i	0.8 (6)
C1i—Ce1i—C9i—C8i	−93.2 (4)	C8i—C7i—C6i—C16i	170.7 (5)
C1i—Ce1i—C9i—C10i	19.9 (4)	C8i—C7i—C6i—Cg2i	0.2 (3)
C1i—Ce1i—C9i—C19i	145.1 (4)	C8i—C7i—Cg2i—C9i	−0.8 (6)
C1i—Ce1i—C9i—Cg2i	−34.7 (4)	C8i—C7i—Cg2i—C10i	178.9 (5)
C1i—Ce1i—Cg1i—C2i	−71.7 (4)	C8i—C9i—Ce1i—Cg1i	−122.9 (3)
C1i—Ce1i—Cg1i—C3i	−143.9 (4)	C8i—C9i—Ce1i—Cg2i	−58.5 (3)
C1i—Ce1i—Cg1i—C4i	144.3 (4)	C8i—C9i—C10i—C20i	−164.1 (5)
C1i—Ce1i—Cg1i—C5i	71.9 (4)	C8i—C9i—C10i—Cg2i	0.8 (3)
C1i—Ce1i—Cg2i—C6i	10.6 (3)	C8i—C9i—Cg2i—C10i	−179.0 (4)
C1i—Ce1i—Cg2i—C7i	−61.4 (3)	C8i—Cg2i—Ce1i—C9i	71.7 (4)
C1i—Ce1i—Cg2i—C8i	−133.9 (3)	C8i—Cg2i—Ce1i—Cg1i	−142.1 (3)
C1i—Ce1i—Cg2i—C9i	154.4 (3)	C8i—Cg2i—C6i—C10i	−179.5 (5)
C1i—Ce1i—Cg2i—C10i	82.1 (3)	C8i—Cg2i—C6i—C16i	−96 (3)
C1i—C2i—Ce1i—C3i	−114.7 (5)	C8i—Cg2i—C7i—C17i	89 (16)
C1i—C2i—Ce1i—C4i	−77.4 (3)	C8i—Cg2i—C9i—C10i	179.0 (4)
C1i—C2i—Ce1i—C5i	−37.1 (3)	C8i—Cg2i—C9i—C19i	97 (9)
C1i—C2i—Ce1i—C6i	75.2 (3)	C8i—Cg2i—C10i—C9i	−1.6 (6)
C1i—C2i—Ce1i—C7i	53.6 (4)	C8i—Cg2i—C10i—C20i	86 (2)
C1i—C2i—Ce1i—C8i	72.8 (4)	C9i—Ce1i—N1i—C21i	88.8 (4)
C1i—C2i—Ce1i—C9i	112.7 (3)	C9i—Ce1i—N1i—C25i	−97.8 (4)
C1i—C2i—Ce1i—Cg1i	−57.4 (3)	C9i—Ce1i—N2i—C26i	76.6 (4)
C1i—C2i—Ce1i—Cg2i	84.1 (3)	C9i—Ce1i—N2i—C30i	−98.5 (4)
C1i—C2i—C3i—C4i	0.2 (6)	C9i—Ce1i—C1i—C11i	30.0 (6)
C1i—C2i—C3i—C13i	−173.2 (6)	C9i—Ce1i—C1i—Cg1i	−151.9 (2)
C1i—C2i—C3i—Cg1i	−0.1 (4)	C9i—Ce1i—C2i—C12i	−8.6 (6)
C1i—C2i—Cg1i—C3i	179.9 (4)	C9i—Ce1i—C2i—Cg1i	170.1 (2)
C1i—C2i—Cg1i—C4i	179.4 (6)	C9i—Ce1i—C3i—C13i	−48.7 (6)
C1i—C2i—Cg1i—C5i	−0.5 (7)	C9i—Ce1i—C3i—Cg1i	133.7 (3)
C1i—C5i—Ce1i—C2i	36.5 (3)	C9i—Ce1i—C4i—Cg1i	111 (1)
C1i—C5i—Ce1i—C3i	75.8 (3)	C9i—Ce1i—C5i—C15i	58.7 (6)
C1i—C5i—Ce1i—C4i	113.0 (5)	C9i—Ce1i—C5i—Cg1i	−119.0 (4)
C1i—C5i—Ce1i—C6i	−43.8 (4)	C9i—Ce1i—C6i—C10i	−34.9 (3)
C1i—C5i—Ce1i—C7i	−75.5 (3)	C9i—Ce1i—C6i—C16i	−160.0 (5)
C1i—C5i—Ce1i—C8i	−96.5 (4)	C9i—Ce1i—C6i—Cg2i	19.8 (2)
C1i—C5i—Ce1i—C9i	−62.8 (5)	C9i—Ce1i—C7i—C17i	160.8 (5)
C1i—C5i—Ce1i—Cg1i	56.2 (3)	C9i—Ce1i—C7i—Cg2i	−19.3 (2)

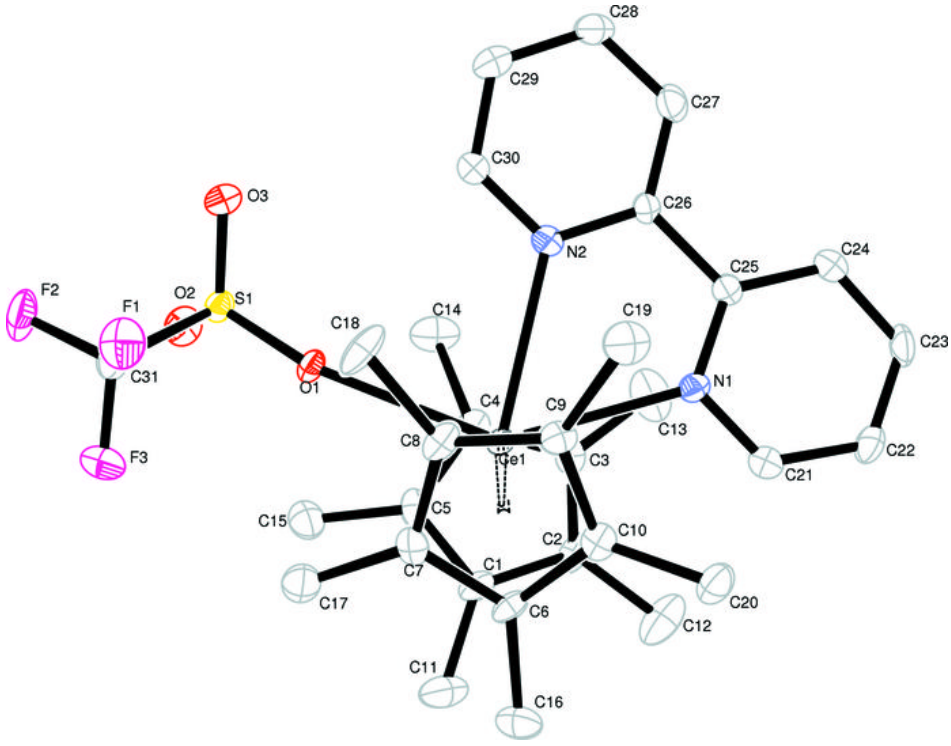
C1i—C5i—Ce1i—Cg2i	−60.4 (4)	C9i—Ce1i—C8i—C18i	123.2 (6)
C1i—C5i—C4i—C3i	0.9 (6)	C9i—Ce1i—C8i—Cg2i	−55.4 (3)
C1i—C5i—C4i—C14i	177.7 (5)	C9i—Ce1i—Cg2i—C10i	−72.3 (4)
C1i—C5i—C4i—Cg1i	0.5 (4)	C9i—C8i—Ce1i—Cg1i	126.8 (3)
C1i—C5i—Cg1i—C2i	0.5 (7)	C9i—C8i—Ce1i—Cg2i	55.4 (3)
C1i—C5i—Cg1i—C3i	179.8 (6)	C9i—C8i—C7i—C17i	−177.3 (5)
C1i—C5i—Cg1i—C4i	−179.4 (4)	C9i—C8i—C7i—Cg2i	0.4 (3)
C1i—Cg1i—Ce1i—C2i	71.7 (4)	C9i—C8i—Cg2i—C10i	1.6 (6)
C1i—Cg1i—Ce1i—C3i	143.9 (4)	C9i—C10i—C6i—C16i	−171.8 (5)
C1i—Cg1i—Ce1i—C4i	−144.3 (4)	C9i—C10i—C6i—Cg2i	−1.0 (3)
C1i—Cg1i—Ce1i—C5i	−71.9 (4)	C9i—Cg2i—Ce1i—Cg1i	146.2 (3)
C1i—Cg1i—Ce1i—C6i	18.9 (3)	C9i—Cg2i—C6i—C10i	1.8 (6)
C1i—Cg1i—Ce1i—C7i	−12.8 (3)	C9i—Cg2i—C6i—C16i	84 (4)
C1i—Cg1i—Ce1i—C8i	−21.6 (4)	C9i—Cg2i—C7i—C17i	88 (16)
C1i—Cg1i—Ce1i—C9i	53.3 (4)	C9i—Cg2i—C8i—C18i	−69 (7)
C1i—Cg1i—Ce1i—Cg2i	17.7 (3)	C9i—Cg2i—C10i—C20i	88 (2)
C1i—Cg1i—C2i—C3i	−179.9 (4)	C10i—C6i—Ce1i—Cg1i	127.1 (3)
C1i—Cg1i—C2i—C12i	82 (4)	C10i—C6i—Ce1i—Cg2i	−54.7 (3)
C1i—Cg1i—C3i—C2i	0.2 (7)	C10i—C6i—C7i—C17i	178.4 (5)
C1i—Cg1i—C3i—C4i	−179.5 (6)	C10i—C6i—C7i—Cg2i	0.7 (3)
C1i—Cg1i—C3i—C13i	109 (5)	C10i—C9i—Ce1i—Cg1i	−9.7 (5)
C1i—Cg1i—C4i—C3i	179.5 (6)	C10i—C9i—Ce1i—Cg2i	54.7 (3)
C1i—Cg1i—C4i—C5i	−0.9 (7)	C10i—C9i—C8i—C18i	174.1 (5)
C1i—Cg1i—C4i—C14i	−70 (13)	C10i—C9i—C8i—Cg2i	−0.8 (3)
C1i—Cg1i—C5i—C4i	179.4 (4)	C10i—Cg2i—Ce1i—Cg1i	73.9 (3)
C1i—Cg1i—C5i—C15i	−73 (3)	C10i—Cg2i—C6i—C16i	82 (3)
C2i—Ce1i—N1i—C21i	−49.8 (4)	C10i—Cg2i—C7i—C17i	−91 (16)
C2i—Ce1i—N1i—C25i	123.7 (4)	C10i—Cg2i—C8i—C18i	−68 (7)
C2i—Ce1i—N2i—C26i	−58.4 (4)	C10i—Cg2i—C9i—C19i	−81 (9)
C2i—Ce1i—N2i—C30i	126.6 (4)	C11i—C1i—Ce1i—Cg1i	−178.1 (6)
C2i—Ce1i—C1i—C5i	−113.5 (5)	C11i—C1i—Ce1i—Cg2i	14.6 (5)
C2i—Ce1i—C1i—C11i	125.7 (6)	C11i—C1i—C2i—C12i	−1.1 (9)
C2i—Ce1i—C1i—Cg1i	−56.2 (3)	C11i—C1i—C2i—Cg1i	169.3 (7)
C2i—Ce1i—C3i—C4i	113.2 (5)	C11i—C1i—C5i—C15i	1.6 (9)
C2i—Ce1i—C3i—C13i	−126.7 (6)	C11i—C1i—C5i—Cg1i	−169.6 (6)
C2i—Ce1i—C3i—Cg1i	55.8 (3)	C12i—C2i—Ce1i—Cg1i	−178.7 (7)
C2i—Ce1i—C4i—C3i	−36.9 (3)	C12i—C2i—Ce1i—Cg2i	−37.2 (5)
C2i—Ce1i—C4i—C5i	75.9 (4)	C12i—C2i—C1i—Cg1i	−170.4 (6)
C2i—Ce1i—C4i—C14i	−161.5 (5)	C12i—C2i—C3i—C13i	−3.0 (9)
C2i—Ce1i—C4i—Cg1i	19.5 (2)	C12i—C2i—C3i—Cg1i	170.1 (6)
C2i—Ce1i—C5i—C4i	−76.5 (3)	C13i—C3i—Ce1i—Cg1i	177.6 (6)
C2i—Ce1i—C5i—C15i	158.0 (5)	C13i—C3i—Ce1i—Cg2i	−95.4 (5)
C2i—Ce1i—C5i—Cg1i	−19.7 (2)	C13i—C3i—C2i—Cg1i	−173.1 (7)
C2i—Ce1i—C6i—C7i	−139.7 (3)	C13i—C3i—C4i—C14i	−3.8 (9)
C2i—Ce1i—C6i—C10i	107.3 (3)	C13i—C3i—C4i—Cg1i	173.4 (6)
C2i—Ce1i—C6i—C16i	−17.9 (5)	C14i—C4i—Ce1i—Cg1i	179.1 (6)
C2i—Ce1i—C6i—Cg2i	162.0 (3)	C14i—C4i—Ce1i—Cg2i	138.4 (4)
C2i—Ce1i—C7i—C6i	47.3 (4)	C14i—C4i—C3i—Cg1i	−177.2 (6)
C2i—Ce1i—C7i—C8i	158.7 (3)	C14i—C4i—C5i—C15i	6.5 (9)

C2i—Ce1i—C7i—C17i	−77.4 (4)	C14i—C4i—C5i—Cg1i	177.3 (6)
C2i—Ce1i—C7i—Cg2i	102.5 (3)	C15i—C5i—Ce1i—Cg1i	177.7 (6)
C2i—Ce1i—C8i—C7i	−34.7 (5)	C15i—C5i—Ce1i—Cg2i	61.1 (5)
C2i—Ce1i—C8i—C9i	77.7 (4)	C15i—C5i—C1i—Cg1i	171.2 (6)
C2i—Ce1i—C8i—C18i	−159.0 (4)	C15i—C5i—C4i—Cg1i	−170.7 (7)
C2i—Ce1i—C8i—Cg2i	22.4 (5)	C16i—C6i—Ce1i—Cg1i	1.9 (5)
C2i—Ce1i—C9i—C8i	−133.2 (3)	C16i—C6i—Ce1i—Cg2i	−179.8 (6)
C2i—Ce1i—C9i—C10i	−20.0 (4)	C16i—C6i—C7i—C17i	−11.7 (9)
C2i—Ce1i—C9i—C19i	105.1 (4)	C16i—C6i—C7i—Cg2i	170.6 (6)
C2i—Ce1i—C9i—Cg2i	−74.7 (3)	C16i—C6i—C10i—C20i	−6.0 (8)
C2i—Ce1i—Cg1i—C3i	−72.2 (4)	C16i—C6i—C10i—Cg2i	−170.8 (6)
C2i—Ce1i—Cg1i—C4i	−144.0 (4)	C17i—C7i—Ce1i—Cg1i	−48.7 (4)
C2i—Ce1i—Cg1i—C5i	143.7 (4)	C17i—C7i—Ce1i—Cg2i	−179.9 (6)
C2i—Ce1i—Cg2i—C6i	−21.1 (3)	C17i—C7i—C6i—Cg2i	177.7 (6)
C2i—Ce1i—Cg2i—C7i	−93.1 (3)	C17i—C7i—C8i—C18i	7.5 (8)
C2i—Ce1i—Cg2i—C8i	−165.6 (3)	C17i—C7i—C8i—Cg2i	−177.7 (6)
C2i—Ce1i—Cg2i—C9i	122.7 (3)	C18i—C8i—Ce1i—Cg1i	−110.0 (4)
C2i—Ce1i—Cg2i—C10i	50.4 (3)	C18i—C8i—Ce1i—Cg2i	178.6 (6)
C2i—C1i—Ce1i—C3i	36.3 (3)	C18i—C8i—C7i—Cg2i	−174.8 (6)
C2i—C1i—Ce1i—C4i	76.0 (4)	C18i—C8i—C9i—C19i	−1.2 (8)
C2i—C1i—Ce1i—C5i	113.5 (5)	C18i—C8i—C9i—Cg2i	175.0 (6)
C2i—C1i—Ce1i—C6i	−106.6 (3)	C19i—C9i—Ce1i—Cg1i	115.4 (4)
C2i—C1i—Ce1i—C7i	−134.4 (3)	C19i—C9i—Ce1i—Cg2i	179.8 (6)
C2i—C1i—Ce1i—C8i	−135.7 (3)	C19i—C9i—C8i—Cg2i	−176.2 (6)
C2i—C1i—Ce1i—C9i	−95.7 (4)	C19i—C9i—C10i—C20i	11.2 (8)
C2i—C1i—Ce1i—Cg1i	56.2 (3)	C19i—C9i—C10i—Cg2i	176.2 (6)
C2i—C1i—Ce1i—Cg2i	−111.1 (3)	C20i—C10i—C6i—Cg2i	164.8 (6)
C2i—C1i—C5i—C4i	−0.8 (6)	C20i—C10i—C9i—Cg2i	−165.0 (6)
C2i—C1i—C5i—C15i	170.9 (5)	C21i—N1i—Ce1i—Cg1i	−68.5 (4)
C2i—C1i—C5i—Cg1i	−0.3 (3)	C21i—N1i—Ce1i—Cg2i	71.5 (4)
C2i—C1i—Cg1i—C3i	−0.2 (7)	C21i—N1i—C25i—C24i	1.6 (8)
C2i—C1i—Cg1i—C4i	−179.4 (6)	C21i—N1i—C25i—C26i	−176.9 (5)
C2i—C1i—Cg1i—C5i	179.7 (4)	C21i—C22i—C23i—C24i	1.7 (9)
C2i—C3i—Ce1i—C4i	−113.2 (5)	C22i—C21i—N1i—C25i	−1.3 (8)
C2i—C3i—Ce1i—C5i	−75.6 (4)	C22i—C23i—C24i—C25i	−1.5 (9)
C2i—C3i—Ce1i—C6i	12.2 (4)	C23i—C24i—C25i—C26i	178.2 (5)
C2i—C3i—Ce1i—C7i	−19.0 (5)	C24i—C25i—C26i—C27i	−6.8 (8)
C2i—C3i—Ce1i—C9i	77.9 (4)	C25i—N1i—Ce1i—Cg1i	105.0 (4)
C2i—C3i—Ce1i—Cg1i	−55.8 (3)	C25i—N1i—Ce1i—Cg2i	−115.0 (4)
C2i—C3i—Ce1i—Cg2i	31.2 (5)	C25i—C26i—N2i—C30i	178.6 (5)
C2i—C3i—C4i—C5i	−0.6 (6)	C25i—C26i—C27i—C28i	−178.1 (5)
C2i—C3i—C4i—C14i	−177.5 (5)	C26i—N2i—Ce1i—Cg1i	−84.9 (4)
C2i—C3i—C4i—Cg1i	−0.2 (3)	C26i—N2i—Ce1i—Cg2i	84.2 (4)
C2i—C3i—Cg1i—C4i	179.7 (4)	C26i—N2i—C30i—C29i	0.4 (9)
C2i—C3i—Cg1i—C5i	−179.5 (6)	C26i—C27i—C28i—C29i	−1.5 (9)
C2i—Cg1i—Ce1i—C3i	72.2 (4)	C27i—C26i—N2i—C30i	−1.2 (8)
C2i—Cg1i—Ce1i—C4i	144.0 (4)	C27i—C28i—C29i—C30i	0.8 (9)
C2i—Cg1i—Ce1i—C5i	−143.7 (4)	C30i—N2i—Ce1i—Cg1i	100.1 (4)
C2i—Cg1i—Ce1i—C6i	−52.9 (3)	C30i—N2i—Ce1i—Cg2i	−90.8 (4)

C2i—Cg1i—Ce1i—C7i	−84.5 (3)	Cg1i—Ce1i—C6i—Cg2i	−178.3 (2)
C2i—Cg1i—Ce1i—C8i	−93.3 (4)	Cg1i—Ce1i—C7i—Cg2i	131.2 (2)
C2i—Cg1i—Ce1i—C9i	−18.4 (4)	Cg1i—Ce1i—C8i—Cg2i	71.5 (4)
C2i—Cg1i—Ce1i—Cg2i	−54.0 (3)	Cg1i—Ce1i—C9i—Cg2i	−64.4 (4)
C2i—Cg1i—C1i—C5i	−179.7 (4)	Cg1i—C1i—Ce1i—Cg2i	−167.3 (2)
C2i—Cg1i—C1i—C11i	−98 (3)	Cg1i—C2i—Ce1i—Cg2i	141.5 (2)
C2i—Cg1i—C3i—C4i	−179.7 (4)	Cg1i—C3i—Ce1i—Cg2i	87.0 (3)
C2i—Cg1i—C3i—C13i	109 (5)	Cg1i—C4i—Ce1i—Cg2i	−40.7 (6)
C2i—Cg1i—C4i—C3i	0.5 (7)	Cg1i—C5i—Ce1i—Cg2i	−116.6 (2)
C2i—Cg1i—C4i—C5i	−180.0 (5)		

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) *x*−1/2, −*y*+1/2, *z*−1/2; (iii) −*x*+1/2, *y*−1/2, −*z*−1/2; (iv) *x*+1/2, −*y*+1/2, *z*−1/2; (v) −*x*+1/2, *y*−1/2, −*z*+1/2; (vi) −*x*+1/2, *y*+1/2, −*z*+1/2.

Fig. 1


C28
C29
C27
C30
O3
C26
N2
C25
C24
F2
F1
O2
S1
C18
C14
C19
C23
C31
O1
N1
C4
C9
C13
C8
Ce1
C3
C22
F3
C21
C15
C5
C2
C10
C7
C1
C17
C6
C20
C12
C11
C16