Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis{4-[(4*H*-1,2,4-triazol-4-yl)iminomethyl]pyridinium} diaquapentanitratocerate(III)

Qiaozhen Sun,* Feng Zheng, Xiaodan Sun and Wei Wang

Department of Materials Chemistry, School of Materials Science and Engineering, Central South University, Changsha, 410083, People's Republic of China
Correspondence e-mail: rosesunqz@yahoo.com.cn

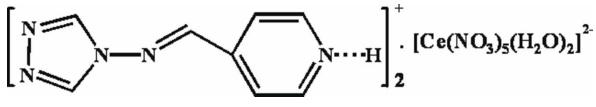
Received 20 September 2008; accepted 18 December 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.024; wR factor = 0.051; data-to-parameter ratio = 10.3.

The asymmetric unit of the title compound, $(C_8H_8N_5)_2[Ce(NO_3)_5(H_2O)_2]$, contains one independent protonated 4-pyridylmethyleneamino-1,2,4-triazole cation and half of a centrosymmetric $[Ce(NO_3)_5(H_2O)_2]^{2-}$ anion. The Ce atom coordinated by five NO_3^- anions and two water molecules, exhibiting a distorted 10-coordination. In the crystal structure, intermolecular O—H···N and N—H···O hydrogen bonds result in the formation of a supramolecular structure.

Related literature

For related compounds based on 4-amido-1,2,4-triazoles Schiff base ligands, see: Drabent *et al.* (2003, 2004); Wang *et al.* (2006). For the preparation of the ligand, see: Colautti *et al.* (1971).



Experimental

Crystal data

$(C_8H_8N_5)_2[Ce(NO_3)_5(H_2O)_2]$
M_r = 834.59
Monoclinic, $C2/c$
a = 10.322 (4) Å
b = 16.126 (6) Å
c = 17.595 (7) Å
β = 100.107 (4)°
V = 2883.2 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.69 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.682, T_{max} = 0.781
5464 measured reflections
2374 independent reflections
2164 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.051
S = 1.02
2374 reflections
231 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
OW1—HW1A···N7	0.85 (2)	1.96 (2)	2.805 (3)	176 (3)
OW1—HW1B···N8^{i}	0.85 (2)	2.03 (3)	2.876 (3)	178 (3)
N4—H4B···O4^{ii}	0.86	1.95	2.804 (3)	172
N4—H4B···N2^{ii}	0.86	2.69	3.518 (4)	162

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors acknowledge financial support from the Innovation Program for College Students of Central South University (grant No. 081053308).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2094).

References

Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Colautti, A., Ferlauto, R. J., Maurich, V., De Nardo, M., Nisi, C., Rubessa, F. & Runti, C. (1971). *Chim. Ther.* **6**, 367–379.
Drabent, K., Bialońska, A. & Ciunik, Z. (2004). *Inorg. Chem. Commun.* **7**, 224–227.
Drabent, K., Ciunik, Z. & Chmielewski, P. J. (2003). *Eur. J. Inorg. Chem.* pp. 1548–1554.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, Y., Yi, L., Yang, X., Ding, B., Cheng, P., Liao, D.-Z. & Yan, S.-P. (2006). *Inorg. Chem.* **45**, 5822–5829.

supporting information

Acta Cryst. (2009). E**65**, m124 [doi:10.1107/S1600536808043109]

Bis{4-[(4*H*-1,2,4-triazol-4-yl)iminomethyl]pyridinium} diaqua-pentanitratocerate(III)

Qiaozhen Sun, Feng Zheng, Xiaodan Sun and Wei Wang

S1. Comment

In recent decades, metal coordination polymers containing 1,2,4-triazoles and their derivatives have been studied widely due to their versatile bridging modes with metal ions. Relatively few structurally characterized compounds based on 4-amido-1,2,4-triazoles Schiff base ligands have been reported (Drabent *et al.*, 2004 and 2003; Wang *et al.*, 2006) and these compounds exhibit dinuclear and tetranuclear structures. In this work, 4-Pyridylmethyleneamino-1,2,4-triazole coordinated with metal cerium is shown to generate a new coordination compound and its crystal structure reported.

As depicted in Fig.1, the Ce ion in this complex is ligated by eight oxygen atoms from five NO_3^- anions and two from H_2O molecules. And three NO_3^- anions are bound to Ce ion in bidentate fashion, while the other two in monodentate one. The nitrogen atoms of Schiff base ligand are not involved in the coordination to the Ce center as we supposed. The $[Ce(NO_3)_5(H_2O)]^{2-}$ unit and the ligands are linked through the O—H···N and N—H···O hydrogen bonds, forming a three dimensional network.

S2. Experimental

The ligand was prepared according to the reported literature (Colautti *et al.*, 1971). The ligand (0.1 mmol, 0.017 g) and $(NH_4)_2Ce(NO_3)_6$ (0.1 mmol, 0.055 g) were mixed in acetonitrile and methanol of 1:1. After stirring at room temperature for four hours, the yellow solution was filtered and evaporated at room temperature. A few days later the red block crystals were obtained.

S3. Refinement

All of the non-hydrogen atoms were refined with anisotropic thermal displacement parameters. The hydrogen atoms on the water coordinated to the Ce atom were located in the difference Fourier, restraints applied to distance and angles and then refined. The positions of other hydrogen atoms were fixed geometrically at calculated distances and allowed to ride on the parent non-hydrogen atoms.

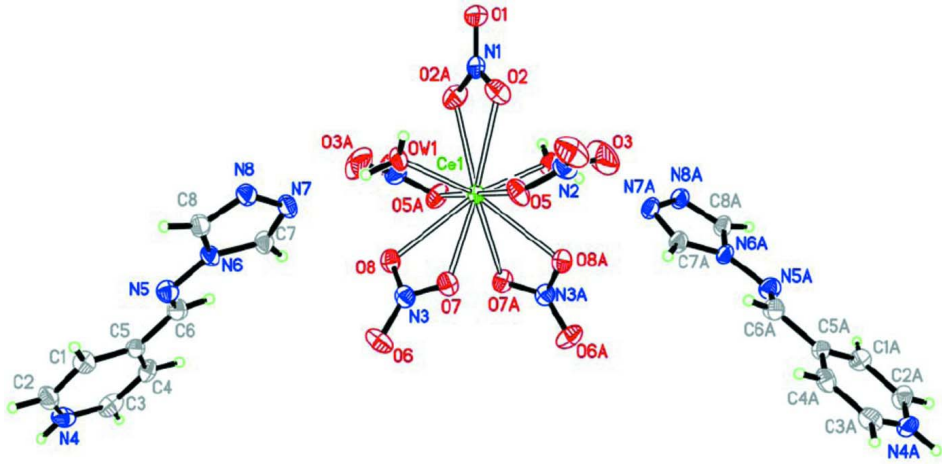


Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [symmetry codes: (A) 1 - *x*, *y*, 0.5 - *z*.]

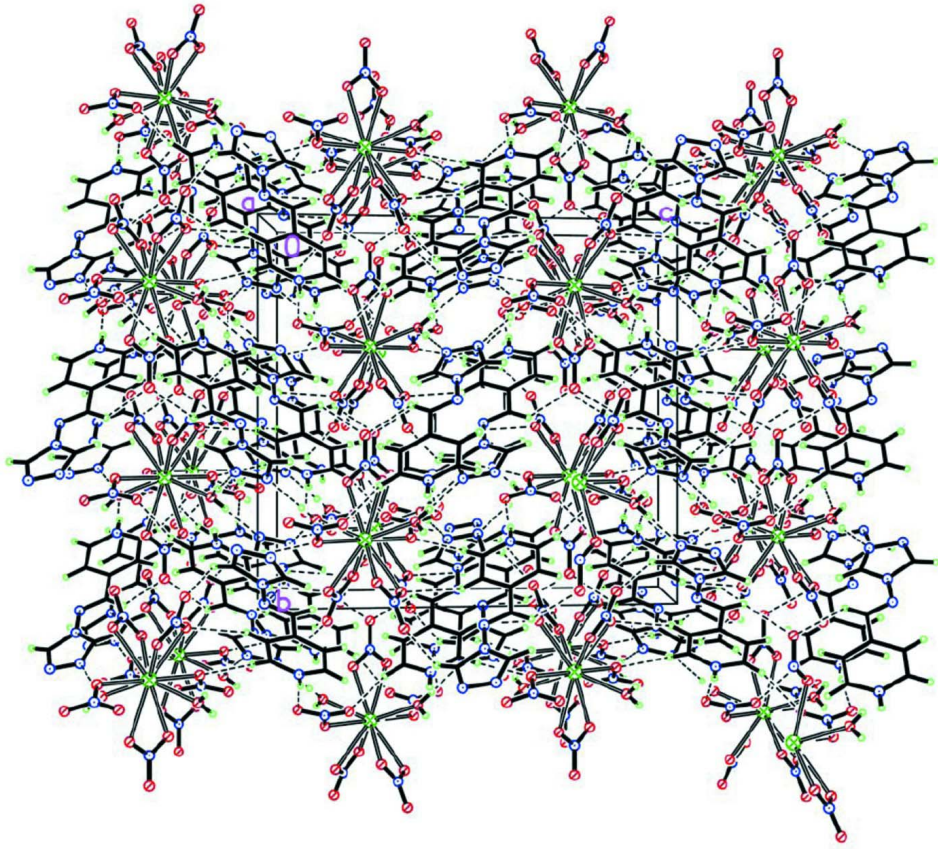


Figure 2

A packing diagram of the title compound along *a* axis. The dash lines indicate hydrogen bonding.

Bis{4-[(4*H*-1,2,4-triazol-4-yl)iminomethyl]pyridinium} diaquapentanitratocerate(III)

Crystal data

$(C_8H_8N_5)_2[Ce(NO_3)_5(H_2O)_2]$
$M_r = 834.59$
Monoclinic, $C2/c$
$a = 10.322$ (4) Å
$b = 16.126$ (6) Å
$c = 17.595$ (7) Å
$\beta = 100.107$ (4)°
$V = 2883.2$ (19) Å^3
$Z = 4$
$F(000) = 1660$
$D_x = 1.923$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4413 reflections
$\theta = 2.4$–27.9°
$\mu = 1.69$ mm^{-1}
$T = 293$ K
Block, red
0.2 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ & ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.682$, $T_{max} = 0.781$
5464 measured reflections
2374 independent reflections
2164 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -8 \rightarrow 12$
$k = -19 \rightarrow 17$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.051$
$S = 1.02$
2374 reflections
231 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: geom, H2O from difmap
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0252P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Special details

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

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ce1	0.5000	0.326614 (13)	0.2500	0.03115 (9)
O1	0.5000	0.0598 (2)	0.2500	0.0705 (10)
O2	0.4319 (2)	0.17726 (13)	0.28901 (13)	0.0562 (6)
O3	0.1789 (3)	0.2766 (2)	0.29302 (17)	0.1053 (11)

O4	0.2177 (3)	0.27312 (16)	0.41595 (15)	0.0779 (8)
O5	0.3593 (2)	0.32656 (13)	0.35615 (12)	0.0503 (5)
O6	0.7035 (2)	0.54285 (14)	0.34535 (13)	0.0652 (7)
O7	0.53719 (19)	0.45902 (12)	0.33599 (10)	0.0453 (5)
O8	0.70260 (19)	0.42680 (12)	0.28267 (11)	0.0448 (5)
OW1	0.6436 (2)	0.27739 (13)	0.37050 (11)	0.0416 (5)
HW1A	0.7155 (19)	0.3003 (18)	0.3907 (15)	0.065 (11)*
HW1B	0.617 (3)	0.2462 (16)	0.4032 (13)	0.063 (11)*
N1	0.5000	0.1364 (2)	0.2500	0.0469 (9)
N2	0.2502 (3)	0.29172 (15)	0.35287 (16)	0.0478 (6)
N3	0.6495 (2)	0.47807 (15)	0.32205 (12)	0.0411 (6)
N4	1.5004 (3)	0.66662 (14)	0.40465 (18)	0.0529 (7)
H4B	1.5642	0.7007	0.4036	0.063*
N5	1.1739 (2)	0.46981 (15)	0.46894 (14)	0.0462 (6)
N6	1.0647 (2)	0.41729 (13)	0.46749 (12)	0.0372 (5)
N7	0.8835 (2)	0.34651 (15)	0.44223 (14)	0.0457 (6)
N8	0.9425 (2)	0.33038 (14)	0.51796 (14)	0.0434 (6)
C1	1.3894 (3)	0.57624 (18)	0.47348 (16)	0.0440 (7)
H1A	1.3802	0.5513	0.5199	0.053*
C2	1.4894 (3)	0.6306 (2)	0.47130 (18)	0.0505 (8)
H2A	1.5495	0.6424	0.5159	0.061*
C3	1.4172 (3)	0.65205 (19)	0.3402 (2)	0.0524 (9)
H3A	1.4272	0.6796	0.2951	0.063*
C4	1.3168 (3)	0.59701 (18)	0.33902 (16)	0.0432 (7)
H4A	1.2594	0.5858	0.2932	0.052*
C5	1.3012 (3)	0.55803 (16)	0.40681 (16)	0.0368 (6)
C6	1.1905 (3)	0.49910 (17)	0.40619 (17)	0.0457 (7)
H6A	1.1356	0.4847	0.3604	0.055*
C7	0.9585 (3)	0.39815 (18)	0.41384 (17)	0.0444 (7)
H7A	0.9418	0.4190	0.3638	0.053*
C8	1.0501 (3)	0.37400 (17)	0.53134 (16)	0.0417 (7)
H8A	1.1085	0.3752	0.5780	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.02878 (14)	0.03952 (14)	0.02512 (12)	0.000	0.00461 (9)	0.000
O1	0.061 (2)	0.043 (2)	0.097 (3)	0.000	−0.015 (2)	0.000
O2	0.0595 (15)	0.0588 (14)	0.0529 (13)	−0.0164 (12)	0.0170 (12)	−0.0075 (11)
O3	0.113 (3)	0.105 (2)	0.077 (2)	−0.0392 (19)	−0.0401 (19)	−0.0047 (17)
O4	0.086 (2)	0.0829 (18)	0.0775 (17)	−0.0295 (15)	0.0491 (16)	−0.0101 (14)
O5	0.0423 (13)	0.0648 (13)	0.0487 (12)	−0.0198 (11)	0.0215 (10)	−0.0070 (10)
O6	0.0732 (17)	0.0559 (14)	0.0640 (15)	−0.0263 (13)	0.0049 (13)	−0.0135 (11)
O7	0.0409 (12)	0.0547 (12)	0.0417 (11)	−0.0040 (10)	0.0107 (10)	−0.0061 (9)
O8	0.0358 (12)	0.0544 (13)	0.0450 (11)	−0.0019 (10)	0.0090 (10)	−0.0021 (10)
OW1	0.0351 (12)	0.0502 (12)	0.0361 (11)	−0.0123 (10)	−0.0035 (10)	0.0090 (10)
N1	0.036 (2)	0.052 (2)	0.047 (2)	0.000	−0.0087 (18)	0.000
N2	0.0502 (18)	0.0448 (14)	0.0493 (16)	−0.0041 (13)	0.0110 (15)	−0.0076 (12)

N3	0.0437 (15)	0.0478 (15)	0.0288 (12)	−0.0036 (13)	−0.0019 (11)	0.0036 (11)
N4	0.0437 (16)	0.0403 (15)	0.080 (2)	−0.0064 (12)	0.0264 (16)	−0.0004 (14)
N5	0.0458 (16)	0.0478 (14)	0.0457 (14)	−0.0041 (12)	0.0101 (12)	0.0040 (12)
N6	0.0311 (13)	0.0360 (12)	0.0440 (14)	−0.0087 (10)	0.0053 (11)	0.0049 (10)
N7	0.0367 (14)	0.0475 (15)	0.0499 (15)	−0.0104 (12)	−0.0008 (12)	0.0030 (11)
N8	0.0391 (14)	0.0423 (13)	0.0472 (14)	−0.0063 (12)	0.0029 (12)	0.0071 (11)
C1	0.0500 (19)	0.0494 (18)	0.0351 (15)	−0.0024 (15)	0.0143 (15)	0.0040 (13)
C2	0.046 (2)	0.0555 (19)	0.0474 (19)	−0.0051 (17)	0.0011 (16)	−0.0111 (16)
C3	0.055 (2)	0.054 (2)	0.056 (2)	0.0130 (17)	0.0306 (19)	0.0225 (16)
C4	0.0393 (18)	0.0563 (18)	0.0335 (15)	0.0104 (15)	0.0046 (14)	0.0039 (13)
C5	0.0314 (16)	0.0354 (15)	0.0449 (16)	0.0002 (13)	0.0105 (14)	−0.0005 (12)
C6	0.0474 (19)	0.0477 (18)	0.0397 (17)	0.0000 (15)	0.0011 (15)	−0.0002 (13)
C7	0.0393 (18)	0.0503 (18)	0.0412 (16)	−0.0034 (15)	0.0000 (15)	0.0071 (14)
C8	0.0376 (17)	0.0434 (17)	0.0419 (16)	−0.0050 (14)	0.0013 (14)	0.0052 (13)

Geometric parameters (Å, º)

Ce1—OW1^{i}	2.494 (2)	N4—C2	1.331 (4)
Ce1—OW1	2.494 (2)	N4—H4B	0.8600
Ce1—O5	2.5590 (19)	N5—C6	1.240 (3)
Ce1—O5^{i}	2.5590 (19)	N5—N6	1.406 (3)
Ce1—O7	2.606 (2)	N6—C7	1.350 (3)
Ce1—O7^{i}	2.606 (2)	N6—C8	1.353 (3)
Ce1—O8	2.625 (2)	N7—C7	1.296 (4)
Ce1—O8^{i}	2.625 (2)	N7—N8	1.389 (3)
Ce1—O2^{i}	2.634 (2)	N8—C8	1.301 (4)
Ce1—O2	2.634 (2)	C1—C2	1.360 (4)
O1—N1	1.235 (5)	C1—C5	1.384 (4)
O2—N1	1.253 (3)	C1—H1A	0.9300
O3—N2	1.199 (3)	C2—H2A	0.9300
O4—N2	1.251 (3)	C3—C4	1.362 (4)
O5—N2	1.251 (3)	C3—H3A	0.9300
O6—N3	1.221 (3)	C4—C5	1.383 (4)
O7—N3	1.264 (3)	C4—H4A	0.9300
O8—N3	1.264 (3)	C5—C6	1.485 (4)
OW1—HW1A	0.849 (10)	C6—H6A	0.9300
OW1—HW1B	0.846 (10)	C7—H7A	0.9300
N1—O2^{i}	1.253 (3)	C8—H8A	0.9300
N4—C3	1.318 (4)		
OW1^{i}—Ce1—OW1	142.88 (10)	N3—O7—Ce1	97.65 (15)
OW1^{i}—Ce1—O5	106.96 (7)	N3—O8—Ce1	96.72 (15)
OW1—Ce1—O5	73.02 (8)	Ce1—OW1—HW1A	124.3 (19)
OW1^{i}—Ce1—O5^{i}	73.02 (8)	Ce1—OW1—HW1B	123.5 (19)
OW1—Ce1—O5^{i}	106.96 (7)	HW1A—OW1—HW1B	109.8 (16)
O5—Ce1—O5^{i}	179.96 (9)	O1—N1—O2	121.74 (18)
OW1^{i}—Ce1—O7	139.41 (7)	O1—N1—O2^{i}	121.74 (18)
OW1—Ce1—O7	76.24 (7)	O2—N1—O2^{i}	116.5 (4)

O5—Ce1—O7	67.74 (6)	O3—N2—O5	122.7 (3)
O5^{i}—Ce1—O7	112.29 (7)	O3—N2—O4	120.8 (3)
OW1^{i}—Ce1—O7^{i}	76.24 (7)	O5—N2—O4	116.5 (3)
OW1—Ce1—O7^{i}	139.41 (7)	O6—N3—O7	121.6 (2)
O5—Ce1—O7^{i}	112.29 (7)	O6—N3—O8	121.8 (2)
O5^{i}—Ce1—O7^{i}	67.74 (6)	O7—N3—O8	116.6 (2)
O7—Ce1—O7^{i}	69.97 (9)	C3—N4—C2	122.5 (3)
OW1^{i}—Ce1—O8	135.54 (6)	C3—N4—H4B	118.8
OW1—Ce1—O8	71.22 (7)	C2—N4—H4B	118.8
O5—Ce1—O8	111.88 (6)	C6—N5—N6	116.7 (3)
O5^{i}—Ce1—O8	68.15 (7)	C7—N6—C8	105.5 (2)
O7—Ce1—O8	48.56 (6)	C7—N6—N5	134.4 (2)
O7^{i}—Ce1—O8	69.72 (6)	C8—N6—N5	120.1 (2)
OW1^{i}—Ce1—O8^{i}	71.22 (6)	C7—N7—N8	107.4 (2)
OW1—Ce1—O8^{i}	135.54 (6)	C8—N8—N7	106.8 (2)
O5—Ce1—O8^{i}	68.15 (7)	C2—C1—C5	120.2 (3)
O5^{i}—Ce1—O8^{i}	111.88 (6)	C2—C1—H1A	119.9
O7—Ce1—O8^{i}	69.72 (6)	C5—C1—H1A	119.9
O7^{i}—Ce1—O8^{i}	48.56 (6)	N4—C2—C1	119.3 (3)
O8—Ce1—O8^{i}	104.04 (9)	N4—C2—H2A	120.4
OW1^{i}—Ce1—O2^{i}	68.49 (7)	C1—C2—H2A	120.4
OW1—Ce1—O2^{i}	77.56 (7)	N4—C3—C4	120.5 (3)
O5—Ce1—O2^{i}	113.68 (7)	N4—C3—H3A	119.7
O5^{i}—Ce1—O2^{i}	66.29 (7)	C4—C3—H3A	119.7
O7—Ce1—O2^{i}	151.86 (7)	C3—C4—C5	119.2 (3)
O7^{i}—Ce1—O2^{i}	128.09 (7)	C3—C4—H4A	120.4
O8—Ce1—O2^{i}	112.40 (7)	C5—C4—H4A	120.4
O8^{i}—Ce1—O2^{i}	138.12 (7)	C4—C5—C1	118.4 (3)
OW1^{i}—Ce1—O2	77.56 (7)	C4—C5—C6	119.4 (3)
OW1—Ce1—O2	68.49 (7)	C1—C5—C6	122.2 (2)
O5—Ce1—O2	66.29 (7)	N5—C6—C5	117.6 (3)
O5^{i}—Ce1—O2	113.68 (7)	N5—C6—H6A	121.2
O7—Ce1—O2	128.09 (7)	C5—C6—H6A	121.2
O7^{i}—Ce1—O2	151.86 (7)	N7—C7—N6	110.1 (2)
O8—Ce1—O2	138.12 (7)	N7—C7—H7A	124.9
O8^{i}—Ce1—O2	112.40 (7)	N6—C7—H7A	124.9
O2^{i}—Ce1—O2	47.72 (10)	N8—C8—N6	110.1 (3)
N1—O2—Ce1	97.88 (19)	N8—C8—H8A	124.9
N2—O5—Ce1	126.02 (17)	N6—C8—H8A	124.9
OW1^{i}—Ce1—O2—N1	72.13 (12)	O7^{i}—Ce1—O8—N3	76.92 (14)
OW1—Ce1—O2—N1	−92.60 (13)	O8^{i}—Ce1—O8—N3	41.97 (12)
O5—Ce1—O2—N1	−172.83 (15)	O2^{i}—Ce1—O8—N3	−159.10 (14)
O5^{i}—Ce1—O2—N1	7.16 (15)	O2—Ce1—O8—N3	−108.18 (15)
O7—Ce1—O2—N1	−143.28 (10)	Ce1—O2—N1—O1	180.0
O7^{i}—Ce1—O2—N1	93.88 (17)	Ce1—O2—N1—O2^{i}	0.0
O8—Ce1—O2—N1	−75.96 (15)	Ce1—O5—N2—O3	−24.5 (4)
O8^{i}—Ce1—O2—N1	135.54 (11)	Ce1—O5—N2—O4	155.8 (2)

O2^{i}—Ce1—O2—N1	0.0	Ce1—O7—N3—O6	173.1 (2)
OW1^{i}—Ce1—O5—N2	14.3 (2)	Ce1—O7—N3—O8	−6.7 (2)
OW1—Ce1—O5—N2	−126.8 (2)	Ce1—O8—N3—O6	−173.2 (2)
O5^{i}—Ce1—O5—N2	−56 (100)	Ce1—O8—N3—O7	6.6 (2)
O7—Ce1—O5—N2	151.4 (2)	C6—N5—N6—C7	−10.8 (4)
O7^{i}—Ce1—O5—N2	96.0 (2)	C6—N5—N6—C8	170.9 (3)
O8—Ce1—O5—N2	172.2 (2)	C7—N7—N8—C8	0.5 (3)
O8^{i}—Ce1—O5—N2	75.3 (2)	C3—N4—C2—C1	0.3 (5)
O2^{i}—Ce1—O5—N2	−59.2 (2)	C5—C1—C2—N4	0.8 (5)
O2—Ce1—O5—N2	−53.4 (2)	C2—N4—C3—C4	−1.6 (5)
OW1^{i}—Ce1—O7—N3	−111.82 (16)	N4—C3—C4—C5	1.6 (4)
OW1—Ce1—O7—N3	80.77 (15)	C3—C4—C5—C1	−0.4 (4)
O5—Ce1—O7—N3	157.79 (16)	C3—C4—C5—C6	178.9 (3)
O5^{i}—Ce1—O7—N3	−22.19 (16)	C2—C1—C5—C4	−0.8 (4)
O7^{i}—Ce1—O7—N3	−76.37 (14)	C2—C1—C5—C6	179.9 (3)
O8—Ce1—O7—N3	3.83 (13)	N6—N5—C6—C5	177.0 (2)
O8^{i}—Ce1—O7—N3	−128.32 (16)	C4—C5—C6—N5	−175.0 (3)
O2^{i}—Ce1—O7—N3	58.9 (2)	C1—C5—C6—N5	4.4 (4)
O2—Ce1—O7—N3	128.58 (14)	N8—N7—C7—N6	−0.2 (3)
OW1^{i}—Ce1—O8—N3	119.31 (14)	C8—N6—C7—N7	−0.1 (3)
OW1—Ce1—O8—N3	−91.83 (15)	N5—N6—C7—N7	−178.6 (3)
O5—Ce1—O8—N3	−29.79 (16)	N7—N8—C8—N6	−0.6 (3)
O5^{i}—Ce1—O8—N3	150.24 (15)	C7—N6—C8—N8	0.5 (3)
O7—Ce1—O8—N3	−3.82 (13)	N5—N6—C8—N8	179.2 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O*W*1—H*W*1*A*···N7	0.85 (2)	1.96 (2)	2.805 (3)	176 (3)
O*W*1—H*W*1*B*···N8^{ii}	0.85 (2)	2.03 (3)	2.876 (3)	178 (3)
N4—H4*B*···O4^{iii}	0.86	1.95	2.804 (3)	172
N4—H4*B*···N2^{iii}	0.86	2.69	3.518 (4)	162

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