data reports

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Crystal structure of μ-peroxido-$\kappa^4O^1,O^2{:}O^{1'},O^{2'}$-bis[(nitrato-$\kappa O$)-(2,2′:6′,2″-terpyridine-κ^3N,N',N'')-dioxidouranium(VI)]

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In the title dimeric complex, [{UO$_2$(NO$_3$)(C$_{15}$H$_{11}$N$_3$)}$_2$O$_2$], a peroxide ion bridges the two uranyl(VI) [O=U=O]$^{2+}$ ions. The O—O bond length of the peroxide is 1.485 (6) Å and the mid-point of this bond is located at the inversion centre of the dimer. The U atom exhibits a distorted hexagonal–bipyramidal coordination geometry with two uranyl(VI) O atoms occupying the axial positions and one O atom of the monodentate nitrate ion, both O atoms of the peroxide ion and the three N atoms of the chelating tridentate 2,2′:6′,2″-terpyridine (terpy) ligand in the equatorial positions. Two of the N atoms of the terpy ligand lie above and below the mean plane containing the equatorial ligand atoms and the U atom [deviations from the mean plane: maximum 0.500 (2), minimum −0.472 (2) and r.m.s. = 0.2910 Å]. The dihedral angle between the terpy ligand and the mean plane is 35.61 (7)°. The bond lengths around the U atom decrease in the order U—N > U—O$_{nitrate}$ > U—O$_{peroxo}$ > U=O. The dimeric complexes pack in a three-dimensional network held together by weak π–π interactions [centroid–centroid distance = 3.659 (3) Å] between pyridyl rings of the terpy ligands in neighbouring dimers, together with intermolecular C—H···O and C—H···π interactions. Weak intramolecular C—H···O interactions are also observed.

1. Related literature

For the structures of uranyl(VI) complexes with terpy, see: Berthet *et al.* (2004). For the structures of uranyl(VI) μ-κ^2:κ^2-peroxide complexes, see:Charushnikova *et al.* (2001); Goff *et al.* (2008); John *et al.* (2004); Sigmon *et al.* (2009); Takao & Ikeda (2010). For the structures of a uranyl(VI) complex with terpy and a uranyl(VI) μ-κ^2:κ^2-peroxide complex, see: Charushnikova & Den Auwer (2004).
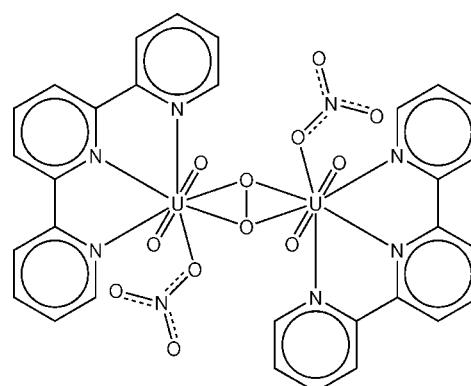
2. Experimental

2.1. Crystal data

[U$_2$(NO$_3$)$_2$(O$_2$)O$_4$(C$_{15}$H$_{11}$N$_3$)$_2$]	V = 1600.0 (2) Å^3
M_r = 1162.62	Z = 2
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 13.4924 (11) Å	μ = 10.19 mm^{-1}
b = 10.2791 (8) Å	T = 90 K
c = 12.6977 (10) Å	0.28 × 0.14 × 0.06 mm
β = 114.691 (1)°	

2.2. Data collection

Bruker APEXII CCD area-detector diffractometer	11692 measured reflections
Absorption correction: analytical (*XPREP*; Bruker, 2007)	4695 independent reflections
T_{min} = 0.163, T_{max} = 0.580	3636 reflections with $I > 2\sigma(I)$
	R_{int} = 0.063

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030	235 parameters
$wR(F^2)$ = 0.058	H-atom parameters constrained
S = 0.89	$\Delta\rho_{max}$ = 2.24 e Å^{-3}
4695 reflections	$\Delta\rho_{min}$ = −1.57 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

U1—O1	1.777 (3)	U1—N2	2.634 (3)
U1—O2	1.775 (3)	U1—N3	2.593 (3)
U1—O3	2.340 (3)	O3—O3^i	1.485 (6)
U1—O3^i	2.325 (3)	O4—N4	1.295 (5)
U1—O4	2.479 (3)	O5—N4	1.232 (5)
U1—N1	2.574 (3)	O6—N4	1.240 (4)
O1—U1—O2	177.31 (13)	O3^i—U1—N1	71.44 (10)
O1—U1—O3	91.64 (14)	O1—U1—N2	76.01 (12)
O1—U1—O3^i	90.58 (14)	O1—U1—N3	100.67 (13)
O1—U1—O4	85.85 (12)	O4—U1—N3	70.03 (11)
O3^i—U1—O3	37.12 (13)	N1—U1—N2	61.29 (11)
O3—U1—O4	66.75 (10)	N2—U1—N3	60.44 (11)
O1—U1—N1	89.42 (13)		

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

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

Cg2 is the centroid of the C6–C10/N2 ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C1—H1⋯O3^i	0.95	2.28	2.773 (6)	112
C1—H1⋯O4^i	0.95	2.59	3.225 (5)	125
C2—H2⋯O6^i	0.95	2.59	3.357 (6)	137
C3—H3⋯O1^{ii}	0.95	2.58	3.176 (6)	121
C4—H4⋯O1^{ii}	0.95	2.55	3.162 (6)	122
C12—H12⋯O5^{iii}	0.95	2.32	3.256 (6)	169
C14—H14⋯O6^{iv}	0.95	2.48	3.246 (7)	138
C15—H15⋯Cg2^v	0.95	2.62	3.512 (5)	157

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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supporting information

Crystal structure of *μ*-peroxido-*κ*⁴*O*¹,*O*²:*O*¹',*O*²'-bis[(nitrato-*κO*)(2,2':6',2''-terpyridine-*κ*³*N*,*N'*,*N''*)dioxidouranium(VI)]

Takeshi Kawasaki and Takafumi Kitazawa

S1. Experimental

10 ml of a methanolic solution containing 0.5 mmol of terpy was added to 10 ml of a methanolic solution containing 0.5 mmol of $UO_2(NO_3)_2 \cdot 6H_2O$ contained in a glass sample vial. The vial w as sealed with a lid and kept in sunlight at room temperature. Yellow crystals grew after one day. The crystal structure of the yellow material has not yet been determined. After about two months, orange crystals of the title complex were obtained.

S2. Refinement

All H atoms were placed at calculated positions, with C(CH)—H = 0.95 Å and allowed to ride on the parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. The (1 0 0) reflection, affected by the beamstop, was omitted from the final refinement.
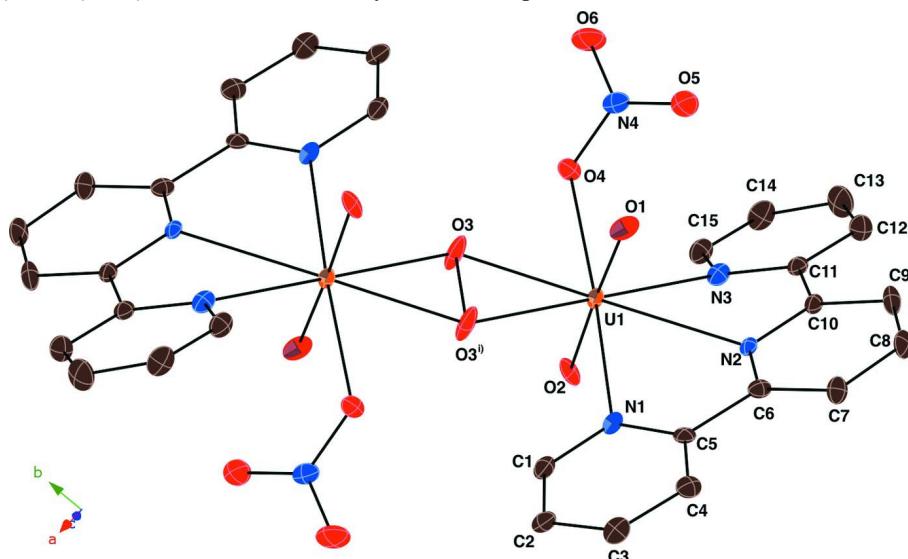

Figure 1

Structure of the dimer [{$UO_2(NO_3)(C_{15}H_{11}N_3)$}$_2O_2$]. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity. [Symmetry code: (i) -x + 1, -y + 1, -z + 1]
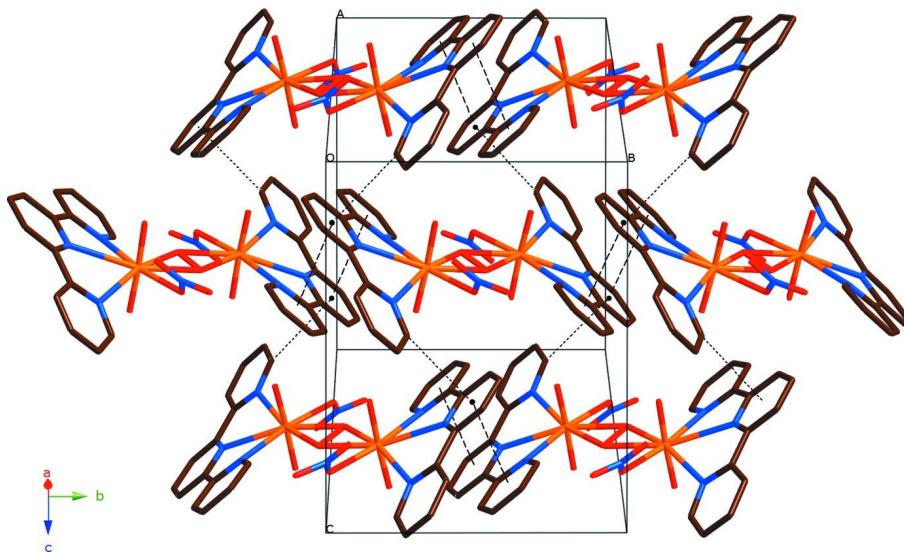
Figure 2

Packing diagram of [{UO₂(NO₃)(C₁₅H₁₁N₃)}₂O₂]. Dashed lines and dotted lines are π–π and C—H⋯π interactions, respectively.

***μ*-Peroxido-*κ⁴O¹,O²:O¹′,O²′*-bis[(nitrato-*κO*)(2,2′:6′,2′′-terpyridine-*κ³N,N′,N′′*)dioxidouranium(VI)]**

Crystal data
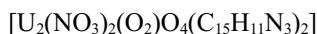
[U₂(NO₃)₂(O₂)O₄(C₁₅H₁₁N₃)₂]	$F(000) = 1076$
$M_r = 1162.62$	$D_x = 2.413$ Mg m⁻³
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 4370 reflections
$a = 13.4924\ (11)$ Å	$\theta = 2.6$–30.1°
$b = 10.2791\ (8)$ Å	$\mu = 10.19$ mm⁻¹
$c = 12.6977\ (10)$ Å	$T = 90$ K
$\beta = 114.691\ (1)°$	Plate, orange
$V = 1600.0\ (2)$ Å³	$0.28 \times 0.14 \times 0.06$ mm
$Z = 2$	

Data collection

Bruker APEXII CCD area-detector diffractometer	11692 measured reflections
Radiation source: fine-focus sealed tube	4695 independent reflections
Graphite monochromator	3636 reflections with $I > 2\sigma(I)$
Detector resolution: 8.333 pixels mm⁻¹	$R_{int} = 0.063$
phi and ω scans	$\theta_{max} = 31.0°$, $\theta_{min} = 2.6°$
Absorption correction: analytical (*XPREP*; Bruker, 2007)	$h = -19 \rightarrow 17$
	$k = -14 \rightarrow 5$
$T_{min} = 0.163$, $T_{max} = 0.580$	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	235 parameters
Least-squares matrix: full	0 restraints
$R[F^2 > 2\sigma(F^2)] = 0.030$	Primary atom site location: structure-invariant direct methods
$wR(F^2) = 0.058$	
$S = 0.89$	Secondary atom site location: difference Fourier map
4695 reflections	

Hydrogen site location: inferred from neighbouring sites	$w = 1/[\sigma^2(F_o^2) + (0.0123P)^2]$

Hydrogen site location: inferred from
  neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0123P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 2.24$ e Å⁻³
$\Delta\rho_{min} = -1.57$ e Å⁻³

Special details

Experimental. face-indexed absorption correction carried out with *XPREP* (Bruker, 2007)

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*	$U_{iso}*/U_{eq}$
U1	0.387048 (13)	0.333645 (14)	0.466857 (14)	0.00993 (5)
O1	0.3311 (3)	0.3633 (3)	0.3151 (3)	0.0176 (7)
O2	0.4441 (3)	0.2963 (3)	0.6171 (3)	0.0168 (7)
O3	0.4596 (3)	0.5439 (3)	0.5073 (4)	0.0306 (10)
O4	0.2546 (2)	0.4979 (3)	0.4721 (3)	0.0152 (6)
O5	0.1152 (3)	0.4243 (3)	0.3199 (3)	0.0242 (8)
O6	0.1038 (3)	0.6064 (3)	0.4006 (3)	0.0283 (9)
N1	0.5298 (3)	0.1823 (3)	0.4461 (3)	0.0126 (7)
N2	0.3249 (3)	0.1020 (3)	0.3740 (3)	0.0097 (7)
N3	0.2240 (3)	0.2190 (3)	0.4857 (3)	0.0129 (7)
N4	0.1554 (3)	0.5090 (4)	0.3945 (3)	0.0165 (8)
C1	0.6361 (4)	0.2172 (4)	0.4933 (4)	0.0142 (9)
H1	0.6585	0.2851	0.5491	0.017*
C2	0.7141 (4)	0.1591 (4)	0.4644 (4)	0.0147 (9)
H2	0.7882	0.1858	0.5006	0.018*
C3	0.6820 (4)	0.0616 (4)	0.3821 (4)	0.0157 (9)
H3	0.7329	0.0226	0.3580	0.019*
C4	0.5733 (3)	0.0215 (4)	0.3351 (4)	0.0146 (9)
H4	0.5494	−0.0468	0.2797	0.018*
C5	0.5008 (3)	0.0823 (4)	0.3700 (4)	0.0109 (8)
C6	0.3841 (3)	0.0422 (4)	0.3258 (4)	0.0116 (8)
C7	0.3392 (4)	−0.0538 (4)	0.2412 (4)	0.0149 (9)
H7	0.3831	−0.0977	0.2103	0.018*
C8	0.2299 (4)	−0.0839 (4)	0.2032 (4)	0.0163 (9)
H8	0.1971	−0.1464	0.1436	0.020*
C9	0.1686 (4)	−0.0219 (4)	0.2529 (4)	0.0164 (9)
H9	0.0934	−0.0415	0.2281	0.020*
C10	0.2192 (3)	0.0695 (4)	0.3396 (4)	0.0108 (8)
C11	0.1638 (4)	0.1318 (4)	0.4050 (4)	0.0118 (8)

C12	0.0579 (4)	0.0988 (4)	0.3906 (4)	0.0173 (10)
H12	0.0148	0.0396	0.3318	0.021*
C13	0.0181 (4)	0.1539 (5)	0.4633 (5)	0.0229 (11)
H13	−0.0543	0.1352	0.4530	0.027*
C14	0.0819 (4)	0.2362 (4)	0.5515 (4)	0.0193 (10)
H14	0.0564	0.2702	0.6052	0.023*
C15	0.1850 (4)	0.2679 (4)	0.5589 (4)	0.0156 (9)
H15	0.2293	0.3261	0.6179	0.019*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
U1	0.01075 (8)	0.00727 (7)	0.01268 (8)	−0.00116 (7)	0.00578 (6)	−0.00132 (7)
O1	0.0249 (18)	0.0142 (15)	0.0175 (17)	0.0044 (14)	0.0126 (15)	0.0039 (13)
O2	0.0163 (16)	0.0199 (15)	0.0080 (16)	0.0007 (14)	−0.0011 (13)	−0.0061 (13)
O3	0.0182 (18)	0.0076 (14)	0.075 (3)	0.0007 (14)	0.028 (2)	−0.0085 (17)
O4	0.0111 (14)	0.0162 (14)	0.0164 (16)	0.0003 (14)	0.0038 (13)	0.0012 (14)
O5	0.0236 (18)	0.0189 (16)	0.023 (2)	0.0019 (15)	0.0024 (16)	−0.0031 (15)
O6	0.0224 (19)	0.0228 (17)	0.034 (2)	0.0124 (16)	0.0064 (17)	−0.0034 (17)
N1	0.0164 (18)	0.0082 (16)	0.0143 (19)	−0.0006 (15)	0.0076 (16)	−0.0001 (14)
N2	0.0126 (17)	0.0074 (15)	0.0074 (17)	−0.0017 (14)	0.0025 (15)	0.0016 (13)
N3	0.0180 (19)	0.0115 (16)	0.0102 (19)	0.0002 (16)	0.0069 (16)	0.0012 (14)
N4	0.0161 (18)	0.0158 (17)	0.017 (2)	0.0033 (18)	0.0066 (16)	0.0043 (17)
C1	0.018 (2)	0.0094 (18)	0.016 (2)	−0.0009 (18)	0.007 (2)	0.0004 (17)
C2	0.016 (2)	0.0102 (18)	0.019 (2)	0.0000 (19)	0.0094 (19)	0.0028 (18)
C3	0.022 (2)	0.016 (2)	0.014 (2)	0.0001 (19)	0.012 (2)	0.0025 (18)
C4	0.018 (2)	0.015 (2)	0.010 (2)	0.0022 (18)	0.0046 (18)	0.0002 (17)
C5	0.013 (2)	0.0101 (18)	0.008 (2)	0.0009 (17)	0.0025 (17)	0.0038 (16)
C6	0.014 (2)	0.0117 (19)	0.009 (2)	0.0030 (17)	0.0043 (18)	0.0006 (16)
C7	0.018 (2)	0.015 (2)	0.013 (2)	−0.0036 (19)	0.0064 (19)	−0.0046 (17)
C8	0.022 (2)	0.014 (2)	0.009 (2)	−0.0040 (19)	0.0031 (19)	−0.0054 (17)
C9	0.016 (2)	0.018 (2)	0.013 (2)	−0.0082 (19)	0.0035 (18)	−0.0031 (18)
C10	0.013 (2)	0.0084 (18)	0.009 (2)	−0.0002 (17)	0.0033 (17)	−0.0006 (16)
C11	0.014 (2)	0.0091 (18)	0.010 (2)	0.0002 (17)	0.0036 (17)	0.0012 (16)
C12	0.017 (2)	0.016 (2)	0.019 (3)	−0.0022 (19)	0.007 (2)	0.0003 (19)
C13	0.014 (2)	0.026 (2)	0.032 (3)	−0.004 (2)	0.013 (2)	−0.002 (2)
C14	0.024 (3)	0.017 (2)	0.023 (3)	−0.001 (2)	0.016 (2)	−0.0033 (19)
C15	0.021 (2)	0.013 (2)	0.013 (2)	−0.0002 (19)	0.0074 (19)	−0.0010 (17)

Geometric parameters (Å, º)

U1—O1	1.777 (3)	C2—H2	0.9500
U1—O2	1.775 (3)	C3—C4	1.395 (6)
U1—O3	2.340 (3)	C3—H3	0.9500
U1—O3^i	2.325 (3)	C4—C5	1.380 (6)
U1—O4	2.479 (3)	C4—H4	0.9500
U1—N1	2.574 (3)	C5—C6	1.492 (6)
U1—N2	2.634 (3)	C6—C7	1.397 (6)

U1—N3	2.593 (3)	C7—C8	1.381 (6)
O3—O3ⁱ	1.485 (6)	C7—H7	0.9500
O3—U1ⁱ	2.325 (3)	C8—C9	1.388 (6)
O4—N4	1.295 (5)	C8—H8	0.9500
O5—N4	1.232 (5)	C9—C10	1.391 (6)
O6—N4	1.240 (4)	C9—H9	0.9500
N1—C1	1.351 (6)	C10—C11	1.476 (6)
N1—C5	1.351 (5)	C11—C12	1.404 (6)
N2—C6	1.342 (5)	C12—C13	1.369 (6)
N2—C10	1.347 (5)	C12—H12	0.9500
N3—C15	1.343 (5)	C13—C14	1.380 (7)
N3—C11	1.348 (5)	C13—H13	0.9500
C1—C2	1.386 (6)	C14—C15	1.393 (6)
C1—H1	0.9500	C14—H14	0.9500
C2—C3	1.380 (6)	C15—H15	0.9500

Cg(C1–C5/N1)···Cg(C6–C10/N2)ⁱⁱ	3.659 (3)

O1—U1—O2	177.31 (13)	N1—C1—H1	118.3
O1—U1—O3	91.64 (14)	C2—C1—H1	118.3
O1—U1—O3ⁱ	90.58 (14)	C3—C2—C1	118.7 (4)
O1—U1—O4	85.85 (12)	C3—C2—H2	120.7
O2—U1—O3	90.58 (14)	C1—C2—H2	120.7
O2—U1—O3ⁱ	90.28 (15)	C2—C3—C4	118.7 (4)
O2—U1—O4	96.43 (12)	C2—C3—H3	120.7
O3ⁱ—U1—O3	37.12 (13)	C4—C3—H3	120.7
O3—U1—O4	66.75 (10)	C5—C4—C3	119.2 (4)
O3ⁱ—U1—O4	103.66 (10)	C5—C4—H4	120.4
O1—U1—N1	89.42 (13)	C3—C4—H4	120.4
O2—U1—N1	88.43 (13)	N1—C5—C4	122.8 (4)
O3—U1—N1	108.56 (10)	N1—C5—C6	115.1 (4)
O3ⁱ—U1—N1	71.44 (10)	C4—C5—C6	122.1 (4)
O4—U1—N1	173.19 (10)	N2—C6—C7	121.7 (4)
O1—U1—N2	76.01 (12)	N2—C6—C5	115.9 (4)
O2—U1—N2	101.52 (12)	C7—C6—C5	122.4 (4)
O3—U1—N2	163.57 (12)	C8—C7—C6	118.9 (4)
O3ⁱ—U1—N2	130.60 (10)	C8—C7—H7	120.5
O4—U1—N2	121.97 (10)	C6—C7—H7	120.5
O1—U1—N3	100.67 (13)	C7—C8—C9	119.4 (4)
O2—U1—N3	78.83 (13)	C7—C8—H8	120.3
O3—U1—N3	133.88 (11)	C9—C8—H8	120.3
O3ⁱ—U1—N3	166.46 (13)	C8—C9—C10	118.7 (4)
O4—U1—N3	70.03 (11)	C8—C9—H9	120.6
N1—U1—N2	61.29 (11)	C10—C9—H9	120.6
N1—U1—N3	115.77 (11)	N2—C10—C9	121.8 (4)
N2—U1—N3	60.44 (11)	N2—C10—C11	115.3 (4)
O3ⁱ—O3—U1ⁱ	72.0 (2)	C9—C10—C11	122.8 (4)
O3ⁱ—O3—U1	70.9 (2)	N3—C11—C12	121.2 (4)

U1ⁱ—O3—U1	142.88 (13)	N3—C11—C10	115.4 (4)
N4—O4—U1	124.6 (3)	C12—C11—C10	123.3 (4)
C1—N1—C5	117.1 (4)	C13—C12—C11	118.4 (4)
C1—N1—U1	119.7 (3)	C13—C12—H12	120.8
C5—N1—U1	121.8 (3)	C11—C12—H12	120.8
C6—N2—C10	119.3 (4)	C12—C13—C14	120.9 (4)
C6—N2—U1	118.7 (3)	C12—C13—H13	119.6
C10—N2—U1	117.7 (3)	C14—C13—H13	119.6
C11—N3—C15	119.2 (4)	C13—C14—C15	117.7 (4)
C11—N3—U1	119.9 (3)	C13—C14—H14	121.2
C15—N3—U1	119.1 (3)	C15—C14—H14	121.2
O4—N4—O5	120.4 (4)	N3—C15—C14	122.4 (4)
O4—N4—O6	116.9 (4)	N3—C15—H15	118.8
O5—N4—O6	122.7 (4)	C14—C15—H15	118.8
N1—C1—C2	123.4 (4)		

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

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C6–C10/N2 ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C1—H1⋯O3ⁱ	0.95	2.28	2.773 (6)	112
C1—H1⋯O4ⁱ	0.95	2.59	3.225 (5)	125
C2—H2⋯O6ⁱ	0.95	2.59	3.357 (6)	137
C3—H3⋯O1ⁱⁱⁱ	0.95	2.58	3.176 (6)	121
C4—H4⋯O1ⁱⁱⁱ	0.95	2.55	3.162 (6)	122
C12—H12⋯O5^{iv}	0.95	2.32	3.256 (6)	169
C14—H14⋯O6^v	0.95	2.48	3.246 (7)	138
C15—H15⋯*Cg*2^{vi}	0.95	2.62	3.512 (5)	157

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

Deviations from Least-squares plane (x,y,z in crystal coordinates).

Least-square plane: 0.0823(0.0118)x - 2.3175(0.0073)y + 11.2072(0.0058)z = 4.4537(0.0040), Rms deviation of fitted atoms = 0.2910.

Atom	Deviation
U1	0.0370(0.0010)
O3	0.0090(0.0041)
O3ⁱ	0.0555(0.0042)
O4	-0.2956(0.0023)
N1	0.1666(0.0024)
N2	-0.4723(0.0024)
N3	0.4999(0.0024)

Symmetric code: (i) -x+1,-y+1,-z+1