Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aquadioxidobis(pentane-2,4-dionato)-uranium(VI) pyrazine solvate

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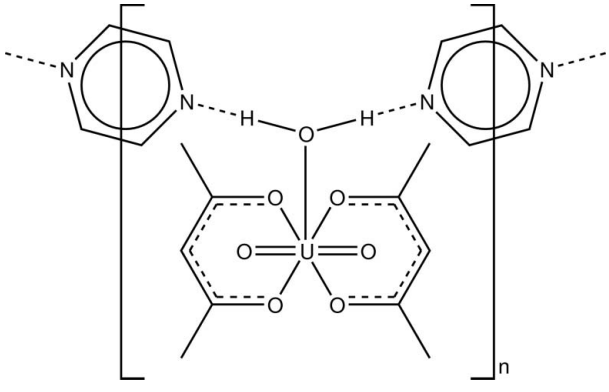
Received 31 March 2008; accepted 3 April 2008

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.009 Å; R factor = 0.032; wR factor = 0.078; data-to-parameter ratio = 19.8.

The asymmetric unit of the title compound, $[U(C_5H_7O_2)_2O_2(H_2O)]\cdot C_4H_4N_2$, contains one $[UO_2(acac)_2(H_2O)]$ (where acac is acetylacetonate) and two half-molecules of pyrazine. It exhibits a UO_7 pentagonal-bipyramidal coordination geometry about the U^{VI} atom, involving two bidentate acetylacetonate ions and one water molecule. The N atoms of the pyrazine molecules are not coordinated to the U^{VI} atom, and are connected with the aqua O atom by hydrogen bonds. This results in a zigzag chain arrangement along the [10$\bar{1}$] direction.

Related literature

For related structures, see: Alcock *et al.* (1984, 1987); Alcock & Flanders (1987); Borkowski & Cahill (2004); Huuskonen *et al.* (2007); Kannan *et al.* (2001); Takao & Ikeda (2008).



Experimental

Crystal data

$[U(C_5H_7O_2)_2O_2(H_2O)]\cdot C_4H_4N_2$
M_r = 566.35
Triclinic, $P\bar{1}$
a = 8.186 (3) Å
b = 8.398 (3) Å
c = 13.663 (4) Å
α = 88.162 (7)°
β = 82.111 (6)°
γ = 86.130 (6)°
V = 928.0 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 8.78 mm^{-1}
T = 299 K
0.22 × 0.14 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.236, T_{max} = 0.590
6928 measured reflections
4526 independent reflections
3841 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.078
S = 1.04
4526 reflections
229 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.63 e Å^{-3}
$\Delta\rho_{min}$ = −1.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

U1—O1	1.777 (3)	U1—O5	2.361 (4)
U1—O2	1.774 (3)	U1—O6	2.353 (3)
U1—O3	2.352 (4)	U1—O7	2.409 (4)
U1—O4	2.348 (4)		
O1—U1—O2	178.98 (14)	O3—U1—O4	70.89 (13)
O1—U1—O3	89.43 (18)	O3—U1—O5	145.58 (15)
O1—U1—O4	90.62 (17)	O3—U1—O6	143.98 (14)
O1—U1—O5	89.85 (18)	O3—U1—O7	72.72 (13)
O1—U1—O6	91.40 (17)	O4—U1—O5	143.53 (13)
O1—U1—O7	90.01 (16)	O4—U1—O6	73.10 (12)
O2—U1—O3	90.37 (17)	O4—U1—O7	143.59 (13)
O2—U1—O4	90.26 (16)	O5—U1—O6	70.43 (13)
O2—U1—O5	89.75 (17)	O5—U1—O7	72.87 (13)
O2—U1—O6	89.35 (16)	O6—U1—O7	143.27 (13)
O2—U1—O7	88.97 (15)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H21···N1	0.86 (4)	1.94 (2)	2.752 (5)	160 (5)
O7—H22···N2	0.85 (4)	1.96 (2)	2.778 (6)	161 (5)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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) and *CrystalMaker* (*CrystalMaker*, 2007); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2447).

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supporting information

Acta Cryst. (2008). E**64**, m673–m674 [doi:10.1107/S1600536808009021]

Aquadioxidobis(pentane-2,4-dionato)uranium(VI) pyrazine solvate

Takeshi Kawasaki and Takafumi Kitazawa

S1. Comment

Actinide chemistry has strong relationship with the reprocessing of nuclear fuels and treatment of actinide wastes in the backend chemistry for the nuclear power plants which operate everyday. The fundamental investigation of the bonding and structure of uranium complexes provides important information on the field of backend chemistry. Various uranyl(VI) complexes with *β*-diketonate have been reported; examples are $[UO_2(acac)_2(H_2O)]$ (Alcock, & Flanders, 1987), $[UO_2(acac)_2(py)]$ (Alcock *et al.*, 1984; Alcock *et al.*, 1987), $[UO_2(tta)_2(H_2O)](H_2O)_2$(dibenzo-18, crown-6) (Kannan *et al.*, 2001), $[UO_2(acac)_2(dmf)]$ (Huuskonen *et al.*, 2007), and $[UO_2(dbm)_2(EtOH)]$ (Takao & Ikeda, 2008). We report herein the synthesis and crystal structure of a new uranyl(VI) acetyl- acetonate complex of formula $[UO_2(acac)_2(H_2O)](pz)$ (**I**) (where acac is acetylacetonate and pz is pyrazine).

The asymmetric unit of the title compound, (I), (Fig. 1), contains one $[UO_2(acac)_2(H_2O)]$ and two-halves of pyrazine molecules. The coordination geometry of the U1 atom has a UO_7 pentagonal-bipyramidal coordination; two uranyl oxygen atoms (O1 and O2) at the axial positions, and the remaining five O atoms from the two chelating acac ligands (O3, O4, O5 and O6) and one H_2O molecule (O7) in the equatorial plane (Table 1). The O1—U1—O2 angle is 178.98 (14) °. The deviations of the O atoms of the acac and of the H_2O from the equatorial plane (O3, O4, O5, O6 and O7) are within 0.02 Å. The U1—O_{acac} bond lengths are longer than the U1—O_{uranyl} distances and are shorter than the U1—O_{aqua} distance. The U1—O7 [2.409 (4) Å] bond is shorter than the U^{VI}—O_{aqua} [2.489 (8) Å] bond of $[UO_2(acac)_2(H_2O)]$ (Alcock, & Flanders, 1987), but similar to the U^{VI}—O_{aqua} [2.396 (5) Å] bond of {$[UO_2(C_9H_4O_6)$- $(H_2O)].H_2O$} (Borkowski & Cahill, 2004) and the U^{VI}—O_{aqua} [2.419 (5) Å] bond of $[UO_2(tta)_2(H_2O)](H_2O)_2$(dibenzo-18,crown-6) (Kannan *et al.*, 2001).

The nitrogen atoms of the pyrazine molecules are not coordinated to the U1, and are connected with O7 atom of the H_2O in the $[UO_2(acac)_2(H_2O)]$ molecule by the hydrogen bonds (Table 2). This results in a zigzag chain arrangement of along the [1 0 - 1] direction (Fig. 2). The dihedral angle between the two pyrazine rings is 13.9 (3)°.

S2. Experimental

To the acetonitrile solution (10 ml) containing $UO_2(NO_3)_2.6H_2O$ (0.5 mmol) was added acetylacetone (3.0 mmol) and pyrazine (3.0 mmol) in acetonitrile (5 ml). After the solvent evaporated slowly at room temperature for a few days, orange crystals of (I) were obtained.

S3. Refinement

H atoms (for H_2O) were located in difference syntheses and refined isotropically by applying restrains on O-H bonds [O-H = 0.852 (10) and 0.849 (10) Å; U_{iso}(H) = 0.062 (16) and 0.069 (18) Å^2]. The remaining H atoms were positioned geometrically, with C-H = 0.93 Å (for CH) and 0.96 Å (for CH_3) and constrained to ride on their parent atoms with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for CH_3 H and x = 1.2 for CH H atoms.

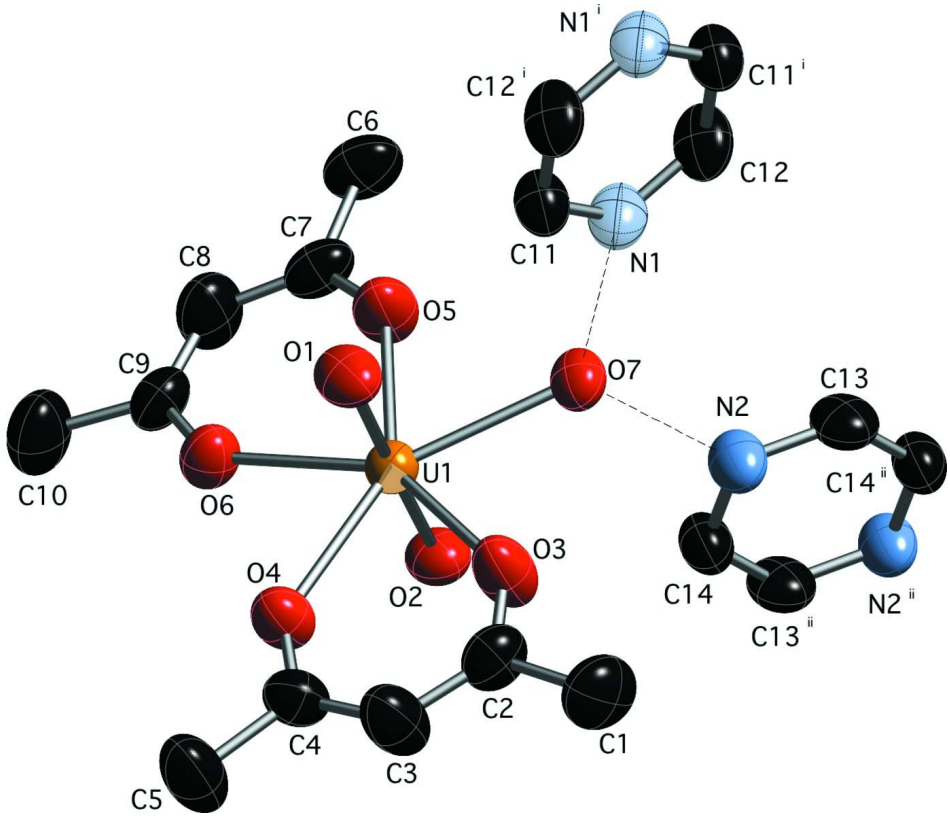

Figure 1

Molecular structure of (I). Displacement ellipsoids are drawn at the 50% probablity level. Hydrogen bonds are shown as dashed lines [symmetry codes: (i) -*x* + 1, -*y* + 2, -*z*; (ii) -*x*, -*y* + 2, -*z* + 1]. H atoms not involved in hydrogen bondings have been omitted for clarity.

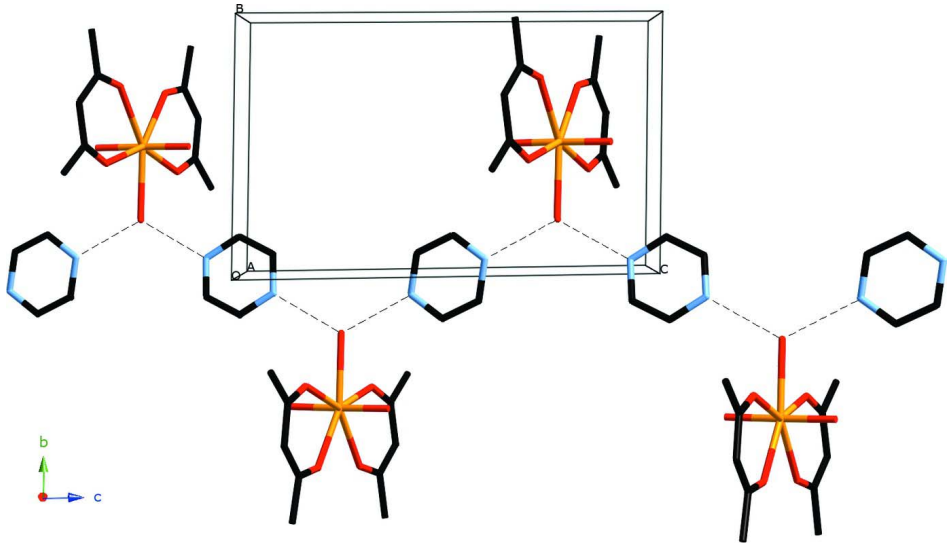

Figure 2

Zigzag chain arragnement formed by O7 of the $[UO_2(acac)_2(H_2O)]$ molecules and the pyrazine molecules in (I). Dashed lines indicate the OH···N hydrogen bonds between neighboring O7 and the pyrazine molecules. H atoms not involved in hydrogen bondings have been omitted for clarity.

Aquadioxidobis(pentane-2,4-dionato)uranium(VI) pyrazine solvate

Crystal data

$[U(C_5H_7O_2)_2O_2(H_2O)]\cdot C_4H_4N_2$
$M_r = 566.35$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.186$ (3) Å
$b = 8.398$ (3) Å
$c = 13.663$ (4) Å
$\alpha = 88.162$ (7)°
$\beta = 82.111$ (6)°
$\gamma = 86.130$ (6)°
$V = 928.0$ (5) Å^3
$Z = 2$
$F(000) = 532$
$D_x = 2.027$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2961 reflections
$\theta = 2.4$–$28.2°$
$\mu = 8.78$ mm^{-1}
$T = 299$ K
Plate, orange
0.22 × 0.14 × 0.06 mm

Data collection

Bruker CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.366 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.236$, $T_{max} = 0.590$
6928 measured reflections
4526 independent reflections
3841 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.5°$
$h = -10\rightarrow10$
$k = -11\rightarrow9$
$l = -18\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.078$
$S = 1.04$
4526 reflections
229 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.5065P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.63$ e Å^{-3}
$\Delta\rho_{min} = -1.27$ 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 $F^2 > 2$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	0.259453 (17)	0.495967 (19)	0.247346 (9)	0.03890 (8)
O1	0.3817 (5)	0.4969 (5)	0.1293 (3)	0.0596 (10)
O2	0.1377 (5)	0.4988 (5)	0.3652 (3)	0.0546 (9)
O3	0.0299 (5)	0.5981 (5)	0.1735 (3)	0.0700 (11)
O4	0.1164 (4)	0.2826 (4)	0.2022 (3)	0.0573 (9)
O5	0.4908 (5)	0.5598 (5)	0.3208 (3)	0.0688 (11)
O6	0.4016 (4)	0.2596 (4)	0.2952 (2)	0.0549 (8)
O7	0.2572 (4)	0.7828 (4)	0.2495 (2)	0.0501 (8)
N1	0.4115 (6)	0.9337 (6)	0.0839 (3)	0.0577 (12)
N2	0.0840 (6)	0.9322 (6)	0.4142 (3)	0.0557 (11)
C1	−0.2101 (7)	0.6668 (8)	0.0993 (5)	0.0789 (19)
H1A	−0.2914	0.7004	0.1534	0.118*
H1B	−0.2637	0.6207	0.0497	0.118*
H1C	−0.1531	0.7573	0.0713	0.118*
C2	−0.0877 (7)	0.5442 (8)	0.1361 (4)	0.0565 (14)
C3	−0.1090 (8)	0.3840 (8)	0.1297 (5)	0.0764 (19)
H3	−0.1992	0.3558	0.1010	0.092*
C4	−0.0086 (6)	0.2633 (7)	0.1619 (4)	0.0547 (12)
C5	−0.0468 (9)	0.0931 (8)	0.1488 (6)	0.088 (2)
H5A	0.0435	0.0399	0.1075	0.133*
H5B	−0.1456	0.0915	0.1184	0.133*
H5C	−0.0625	0.0393	0.2121	0.133*
C6	0.7166 (7)	0.5944 (8)	0.4048 (4)	0.0721 (17)
H6A	0.8071	0.6143	0.3543	0.108*

H6B	0.7580	0.5415	0.4605	0.108*
H6C	0.6591	0.6939	0.4249	0.108*
C7	0.5996 (6)	0.4899 (8)	0.3648 (4)	0.0541 (14)
C8	0.6166 (8)	0.3245 (9)	0.3785 (5)	0.0744 (18)
H8	0.6979	0.2833	0.4152	0.089*
C9	0.5220 (6)	0.2191 (7)	0.3416 (4)	0.0547 (12)
C10	0.5580 (9)	0.0434 (8)	0.3557 (5)	0.086 (2)
H10A	0.4673	−0.0008	0.3974	0.128*
H10B	0.6569	0.0252	0.3860	0.128*
H10C	0.5730	−0.0068	0.2927	0.128*
C11	0.4593 (7)	0.8497 (7)	0.0033 (4)	0.0535 (13)
H11	0.4348	0.7432	0.0030	0.064*
C12	0.4551 (8)	1.0829 (8)	0.0803 (4)	0.0614 (15)
H12	0.4272	1.1446	0.1362	0.074*
C13	0.0714 (7)	1.0896 (7)	0.4270 (4)	0.0569 (14)
H13	0.1206	1.1556	0.3771	0.068*
C14	0.0118 (7)	0.8421 (7)	0.4888 (4)	0.0527 (12)
H14	0.0181	0.7317	0.4833	0.063*
H22	0.202 (6)	0.846 (5)	0.291 (3)	0.069 (18)*
H21	0.284 (6)	0.845 (5)	0.200 (3)	0.062 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
U1	0.04099 (10)	0.04129 (13)	0.03434 (9)	−0.00227 (7)	−0.00502 (6)	−0.00051 (7)
O1	0.069 (2)	0.061 (3)	0.0440 (18)	−0.0096 (19)	0.0121 (16)	−0.0057 (17)
O2	0.058 (2)	0.056 (2)	0.0461 (17)	−0.0055 (18)	0.0052 (15)	0.0023 (17)
O3	0.077 (3)	0.050 (3)	0.091 (3)	−0.004 (2)	−0.043 (2)	0.007 (2)
O4	0.060 (2)	0.052 (2)	0.064 (2)	−0.0073 (17)	−0.0236 (16)	0.0040 (18)
O5	0.058 (2)	0.059 (3)	0.097 (3)	−0.0040 (19)	−0.036 (2)	0.000 (2)
O6	0.0554 (19)	0.053 (2)	0.0590 (19)	0.0022 (17)	−0.0185 (15)	−0.0024 (17)
O7	0.058 (2)	0.046 (2)	0.0426 (17)	0.0002 (17)	0.0050 (15)	−0.0020 (16)
N1	0.065 (3)	0.054 (3)	0.048 (2)	0.004 (2)	0.0087 (19)	0.007 (2)
N2	0.064 (3)	0.050 (3)	0.047 (2)	−0.004 (2)	0.0117 (19)	−0.004 (2)
C1	0.067 (4)	0.082 (5)	0.091 (4)	0.008 (3)	−0.031 (3)	0.015 (4)
C2	0.050 (3)	0.071 (4)	0.049 (3)	0.002 (3)	−0.016 (2)	0.007 (3)
C3	0.067 (4)	0.067 (5)	0.104 (5)	−0.012 (3)	−0.043 (3)	0.009 (4)
C4	0.055 (3)	0.056 (3)	0.056 (3)	−0.014 (2)	−0.013 (2)	0.002 (2)
C5	0.087 (4)	0.060 (4)	0.129 (6)	−0.018 (4)	−0.047 (4)	−0.003 (4)
C6	0.052 (3)	0.097 (5)	0.072 (3)	−0.011 (3)	−0.020 (3)	−0.013 (3)
C7	0.040 (2)	0.080 (4)	0.043 (2)	−0.002 (3)	−0.0084 (18)	−0.007 (3)
C8	0.065 (3)	0.073 (5)	0.091 (4)	0.008 (3)	−0.036 (3)	0.004 (4)
C9	0.044 (2)	0.062 (4)	0.056 (3)	0.011 (2)	−0.006 (2)	0.000 (2)
C10	0.090 (5)	0.065 (4)	0.105 (5)	0.016 (4)	−0.036 (4)	0.001 (4)
C11	0.067 (3)	0.043 (3)	0.048 (3)	0.000 (2)	−0.002 (2)	−0.001 (2)
C12	0.087 (4)	0.055 (4)	0.037 (2)	0.005 (3)	0.006 (2)	−0.007 (2)
C13	0.064 (3)	0.055 (4)	0.048 (3)	−0.013 (3)	0.008 (2)	0.007 (2)
C14	0.062 (3)	0.039 (3)	0.055 (3)	−0.004 (2)	0.001 (2)	−0.001 (2)

Geometric parameters (Å, º)

U1—O1	1.777 (3)	C4—C5	1.505 (8)
U1—O2	1.774 (3)	C5—H5A	0.9600
U1—O3	2.352 (4)	C5—H5B	0.9600
U1—O4	2.348 (4)	C5—H5C	0.9600
U1—O5	2.361 (4)	C6—C7	1.507 (8)
U1—O6	2.353 (3)	C6—H6A	0.9600
U1—O7	2.409 (4)	C6—H6B	0.9600
O3—C2	1.265 (6)	C6—H6C	0.9600
O4—C4	1.249 (6)	C7—C8	1.396 (9)
O5—C7	1.246 (6)	C8—C9	1.366 (8)
O6—C9	1.266 (6)	C8—H8	0.9300
O7—H21	0.86 (4)	C9—C10	1.496 (8)
O7—H22	0.85 (4)	C10—H10A	0.9600
N1—C11	1.326 (7)	C10—H10B	0.9600
N1—C12	1.323 (8)	C10—H10C	0.9600
N2—C13	1.334 (8)	C11—C12^{i}	1.381 (7)
N2—C14	1.344 (6)	C11—H11	0.9300
C1—C2	1.511 (8)	C12—C11^{i}	1.381 (7)
C1—H1A	0.9600	C12—H12	0.9300
C1—H1B	0.9600	C13—C14^{ii}	1.375 (8)
C1—H1C	0.9600	C13—H13	0.9300
C2—C3	1.376 (9)	C14—C13^{ii}	1.375 (8)
C3—C4	1.361 (8)	C14—H14	0.9300
C3—H3	0.9300		
O1—U1—O2	178.98 (14)	O4—C4—C3	124.6 (5)
O1—U1—O3	89.43 (18)	O4—C4—C5	116.1 (5)
O1—U1—O4	90.62 (17)	C3—C4—C5	119.3 (5)
O1—U1—O5	89.85 (18)	C4—C5—H5A	109.5
O1—U1—O6	91.40 (17)	C4—C5—H5B	109.5
O1—U1—O7	90.01 (16)	H5A—C5—H5B	109.5
O2—U1—O3	90.37 (17)	C4—C5—H5C	109.5
O2—U1—O4	90.26 (16)	H5A—C5—H5C	109.5
O2—U1—O5	89.75 (17)	H5B—C5—H5C	109.5
O2—U1—O6	89.35 (16)	C7—C6—H6A	109.5
O2—U1—O7	88.97 (15)	C7—C6—H6B	109.5
O3—U1—O4	70.89 (13)	H6A—C6—H6B	109.5
O3—U1—O5	145.58 (15)	C7—C6—H6C	109.5
O3—U1—O6	143.98 (14)	H6A—C6—H6C	109.5
O3—U1—O7	72.72 (13)	H6B—C6—H6C	109.5
O4—U1—O5	143.53 (13)	O5—C7—C8	123.7 (5)
O4—U1—O6	73.10 (12)	O5—C7—C6	116.4 (6)
O4—U1—O7	143.59 (13)	C8—C7—C6	119.9 (5)
O5—U1—O6	70.43 (13)	C9—C8—C7	124.5 (5)
O5—U1—O7	72.87 (13)	C9—C8—H8	117.7
O6—U1—O7	143.27 (13)	C7—C8—H8	117.7

C2—O3—U1	137.8 (4)	O6—C9—C8	124.2 (5)
C4—O4—U1	137.9 (4)	O6—C9—C10	116.0 (5)
C7—O5—U1	138.5 (4)	C8—C9—C10	119.9 (5)
C9—O6—U1	138.2 (4)	C9—C10—H10A	109.5
U1—O7—H22	129 (4)	C9—C10—H10B	109.5
U1—O7—H21	127 (4)	H10A—C10—H10B	109.5
H22—O7—H21	102 (5)	C9—C10—H10C	109.5
C12—N1—C11	116.2 (4)	H10A—C10—H10C	109.5
C13—N2—C14	116.4 (5)	H10B—C10—H10C	109.5
C2—C1—H1A	109.5	N1—C11—C12^{i}	121.4 (5)
C2—C1—H1B	109.5	N1—C11—H11	119.3
H1A—C1—H1B	109.5	C12^{i}—C11—H11	119.3
C2—C1—H1C	109.5	N1—C12—C11^{i}	122.4 (5)
H1A—C1—H1C	109.5	N1—C12—H12	118.8
H1B—C1—H1C	109.5	C11^{i}—C12—H12	118.8
O3—C2—C3	123.5 (5)	N2—C13—C14^{ii}	122.5 (5)
O3—C2—C1	116.3 (6)	N2—C13—H13	118.8
C3—C2—C1	120.2 (5)	C14^{ii}—C13—H13	118.8
C4—C3—C2	125.3 (5)	N2—C14—C13^{ii}	121.1 (5)
C4—C3—H3	117.3	N2—C14—H14	119.5
C2—C3—H3	117.3	C13^{ii}—C14—H14	119.5

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $-x, -y+2, -z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H21···N1	0.86 (4)	1.94 (2)	2.752 (5)	160 (5)
O7—H22···N2	0.85 (4)	1.96 (2)	2.778 (6)	161 (5)