# Poly[(μ₂-2-hydroxy-2-methylpropionato-κ³O¹,O²:O¹)(μ₂-2-hydroxy-2-methyl-propionato-κ²O¹:κO¹')dioxido-uranium(VI)]

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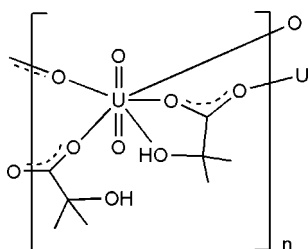Correspondence e-mail: tyoshi@chem.sci.osaka-u.ac.jp

In the title compound, $[UO_2(C_4H_7O_3)_2]_n$, the dioxouranium-(VI) units are linked by 2-hydroxy-2-methylpropionate ligands into a honeycomb structure. The U atom is seven-coordinate in a pentagonal-bipyramidal geometry. The uncoordinated hydroxy groups of the 2-hydroxy-2-methyl-propionate ions interact with the O atom of the uranyl and with the coordinated hydroxy group of an adjacent 2-hydroxy-2-methylpropionate ion through O—H⋯O hydrogen bonds.

## Related literature

For related structures, see: Back *et al.* (2007); Bombieri *et al.* (1973, 1974); Jiang *et al.* (2002); Thuéry (2006, 2007*a,b,c,* 2008); Xie *et al.* (2003); Yokoyama *et al.* (1990).



## Experimental

### Crystal data

| | |
|---|---|
| $[U(C_4H_7O_3)_2O_2]$ | $V$ = 1289.0 (6) Å³ |
| $M_r$ = 476.22 | $Z$ = 4 |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| $a$ = 9.009 (2) Å | $\mu$ = 12.62 mm⁻¹ |
| $b$ = 8.237 (2) Å | $T$ = 200 K |
| $c$ = 17.552 (6) Å | 0.20 × 0.11 × 0.03 mm |
| $\beta$ = 98.246 (9)° | |

### Data collection

| | |
|---|---|
| Rigaku R-AXIS RAPID Imaging Plate diffractometer | 11887 measured reflections |
| Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) | 2949 independent reflections |
| $T_{min}$ = 0.233, $T_{max}$ = 0.685 | 2547 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.050 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.029 | 160 parameters |
| $wR(F^2)$ = 0.100 | H-atom parameters constrained |
| $S$ = 0.86 | $\Delta\rho_{max}$ = 0.99 e Å⁻³ |
| 2949 reflections | $\Delta\rho_{min}$ = −2.15 e Å⁻³ |

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| U1—O1 | 1.783 (5) | U1—O5$^i$ | 2.355 (4) |
| U1—O2 | 1.762 (6) | U1—O7 | 2.346 (5) |
| U1—O3 | 2.444 (5) | U1—O7 | 2.336 (5) |
| U1—O4 | 2.407 (5) | | |

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

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| O3—H13⋯O6 | 0.82 | 1.93 | 2.597 (6) | 138 |
| O6—H14⋯O1$^{ii}$ | 0.82 | 2.00 | 2.777 (6) | 158 |

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *TEXSAN* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *TEXSAN*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2546).

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# supporting information

# Poly[(*μ*₂-2-hydroxy-2-methylpropionato-*κ*³*O*¹,*O*²:*O*¹′)(*μ*₂-2-hydroxy-2-methyl-propionato-*κ*²*O*¹:*κO*¹′)dioxidouranium(VI)]

**Takashi Yoshimura, Hidetoshi Kikunaga and Atsushi Shinohara**

### S1. Comment

Structural chemistry of uranyl(VI) complexes with hydroxycarboxylate or alkoxycarboxylate has been extensively studied (Back *et al.* (2007); Bombieri *et al.*(1973, 1974); Jiang *et al.* (2002); Thuéry (2006, 2007*a*,*b*,*c*, 2008); Xie *et al.* (2003; Yokoyama *et al.*(1990)). The crystals of the title compound (**I**) suitable for single-crystal X-ray analysis were obtained by the reaction of bis(acetato)dioxouranium dihydrate with an excess amount of 2-hydroxy-2-methylpropionic acid in water. Herein, we report on the crystal structure of **I**. Uranium(VI) atom is seven-coordinate in a pentagonal-bipyramidal structure. The two oxygen atoms are located at the axial positions with nearly linear O(1)—U(1)—O(2) angle (178.3 (2)°). The equatorial positions are coordinated by five oxygen atoms of 2-hydroxy-2-methylpropionate (HIB) ligands. Two kinds of HIB ligands exist in the asymmetric unit. One of the HIB ligands links two uranium atoms by the carboxyl group. The other chelates one uranium atom through the hydroxy and carboxyl groups, moreover the carboxyl group bridges the neighboring uranium atom. As a result, a two-dimensional honeycomb structure is formed. The IR spectrum of **I** shows stretching bands of the carboxyl group of HIB at 1614 and 1561 cm⁻¹.

### S2. Experimental

2-Hydroxy-2-methylpropionic acid (150 mg, 1.45 mmol) was added to a solution of bis(acetato)dioxouranium dihydrate (50 mg, 0.12 mmol) in 3 ml of water. The resulting yellow solution was left for several days at room temperature to give yellow crystals, which were filtered off, washed with a small amount of water, and then dried in air.

### S3. Refinement

H atoms bonded to C and O atoms were placed at calculated positions [C—H = 0.96 and O—H = 0.82] and refined as riding with $U_{iso}(H) = 1.0 \ U_{eq}(C,O)$. The deepest hole is 0.68 Å from atom U(1).
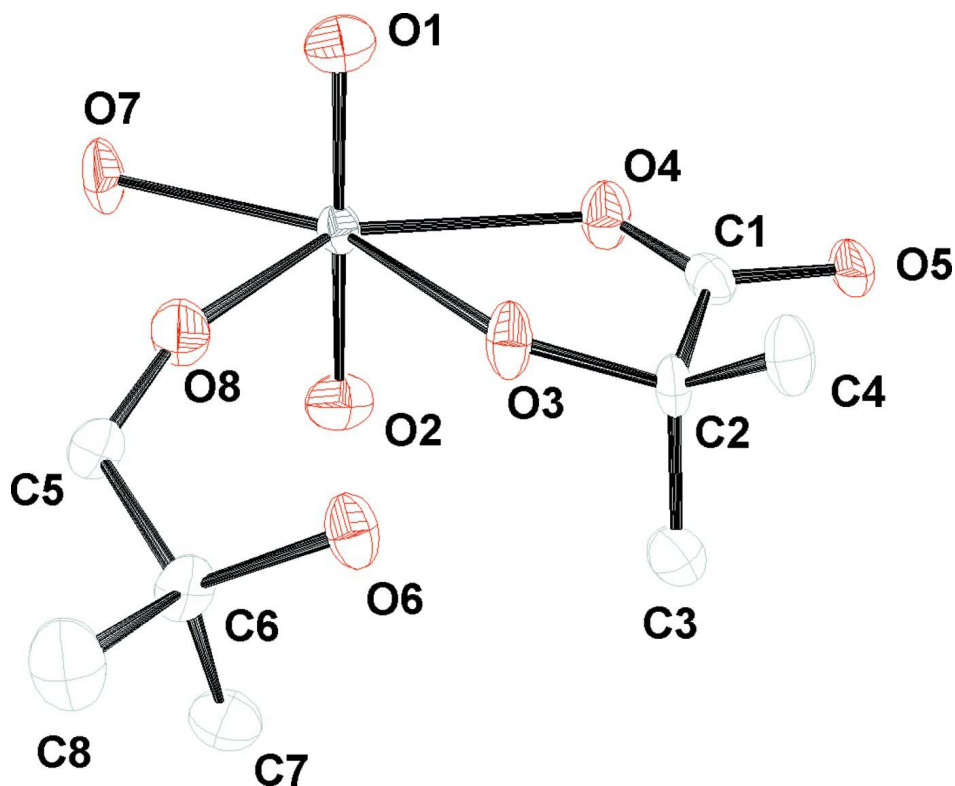
**Figure 1**

The assymmetric unit of **I**, with the atom-numbering scheme and displacement ellipsoids drawn at 50% probability level. Hydrogen atoms are omitted for clarity.
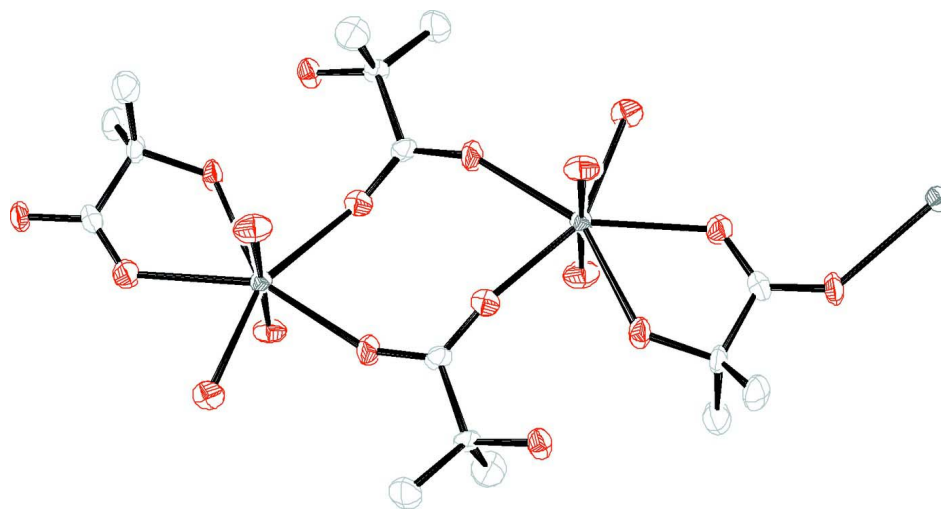


**Figure 2**

Fragment of the polymeric structure. Hydrogen atoms are omitted for clarity.
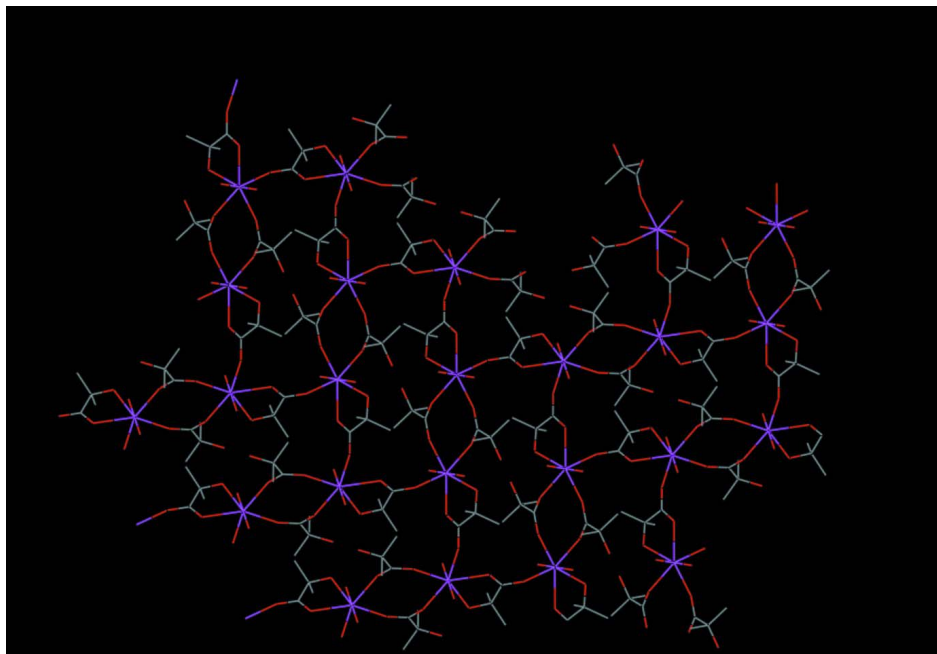
**Figure 3**

View of the polymeric structure. Hydrogen atoms are omitted for clarity.

**Poly[($\mu_2$-2-hydroxy-2-methylpropionato- $\kappa^3O^1$,$O^2$:$O^{1'}$)($\mu_2$-2-hydroxy-2- methylpropionato-$\kappa^2O^1$:$\kappa O^{1'}$)dioxidouranium(VI)]**

*Crystal data*

| | |
|---|---|
| [U(C$_4$H$_7$O$_3$)$_2$O$_2$] | $F(000) = 872.00$ |
| $M_r = 476.22$ | $D_x = 2.454$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å |
| Hall symbol: -P 2yn | Cell parameters from 8716 reflections |
| $a = 9.009$ (2) Å | $\theta = 3.0$–$27.5°$ |
| $b = 8.237$ (2) Å | $\mu = 12.62$ mm$^{-1}$ |
| $c = 17.552$ (6) Å | $T = 200$ K |
| $\beta = 98.246$ (9)° | Platelet, yellow |
| $V = 1289.0$ (6) Å$^3$ | $0.20 \times 0.11 \times 0.03$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID Imaging Plate diffractometer | 11887 measured reflections |
| Radiation source: fine-focus sealed tube | 2949 independent reflections |
| Graphite monochromator | 2547 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 10.00 pixels mm$^{-1}$ | $R_{int} = 0.050$ |
| $\omega$ scans | $\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$ |
| Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) | $h = 12 \rightarrow 11$ |
| | $k = -9 \rightarrow 10$ |
| $T_{min} = 0.233$, $T_{max} = 0.685$ | $l = -22 \rightarrow 22$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.029$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.100$ | |
| $S = 0.86$ | H-atom parameters constrained |
| 2949 reflections | $w = 1/[\sigma^2(F_o^2) + (0.079P)^2 + 5.354P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 160 parameters | |
| Primary atom site location: structure-invariant direct methods | $(\Delta/\sigma)_{max} = 0.001$ |
| | $\Delta\rho_{max} = 0.99$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -2.15$ 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| U(1) | 0.63772 (2) | 0.19668 (3) | 0.62425 (1) | 0.0180 (1) |
| O(1) | 0.7538 (6) | 0.3101 (5) | 0.5695 (3) | 0.028 (1) |
| O(2) | 0.5188 (6) | 0.0891 (6) | 0.6778 (3) | 0.032 (1) |
| O(3) | 0.4753 (5) | 0.4342 (5) | 0.6250 (3) | 0.026 (1) |
| O(4) | 0.6920 (5) | 0.3869 (6) | 0.7286 (3) | 0.029 (1) |
| O(5) | 0.6435 (5) | 0.6018 (6) | 0.7991 (3) | 0.0252 (10) |
| O(6) | 0.2338 (5) | 0.4208 (5) | 0.5248 (3) | 0.0241 (10) |
| O(7) | 0.7009 (6) | −0.0415 (6) | 0.5630 (3) | 0.034 (1) |
| O(8) | 0.4514 (6) | 0.1975 (5) | 0.5169 (3) | 0.030 (1) |
| C(1) | 0.6115 (7) | 0.5015 (8) | 0.7435 (3) | 0.022 (1) |
| C(2) | 0.4611 (7) | 0.5295 (8) | 0.6929 (4) | 0.021 (1) |
| C(3) | 0.3351 (8) | 0.463 (1) | 0.7324 (4) | 0.036 (2) |
| C(4) | 0.4392 (10) | 0.7064 (7) | 0.6704 (5) | 0.030 (2) |
| C(5) | 0.3241 (7) | 0.1601 (8) | 0.4820 (4) | 0.020 (1) |
| C(6) | 0.1889 (7) | 0.2626 (8) | 0.4949 (4) | 0.021 (1) |
| C(7) | 0.1191 (10) | 0.1790 (9) | 0.5588 (5) | 0.039 (2) |
| C(8) | 0.0781 (10) | 0.280 (1) | 0.4211 (5) | 0.038 (2) |
| H(1) | 0.3277 | 0.5253 | 0.7779 | 0.0356* |
| H(2) | 0.2423 | 0.4698 | 0.6980 | 0.0356* |
| H(3) | 0.3555 | 0.3516 | 0.7462 | 0.0356* |
| H(4) | 0.4388 | 0.7711 | 0.7159 | 0.0297* |
| H(5) | 0.3454 | 0.7192 | 0.6374 | 0.0297* |
| H(6) | 0.5196 | 0.7409 | 0.6438 | 0.0297* |
| H(7) | 0.0321 | 0.2384 | 0.5684 | 0.0386* |
| H(8) | 0.1908 | 0.1757 | 0.6048 | 0.0386* |

| | | | | |
|---|---|---|---|---|
| H(9) | 0.0907 | 0.0703 | 0.5432 | 0.0386* |
| H(10) | −0.0100 | 0.3359 | 0.4322 | 0.0383* |
| H(11) | 0.0507 | 0.1746 | 0.4007 | 0.0383* |
| H(12) | 0.1237 | 0.3413 | 0.3841 | 0.0383* |
| H(13) | 0.4210 | 0.4724 | 0.5878 | 0.0255* |
| H(14) | 0.2178 | 0.4883 | 0.4902 | 0.0241* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| U(1) | 0.0192 (2) | 0.0158 (2) | 0.0185 (2) | 0.00083 (8) | 0.0005 (1) | −0.00114 (8) |
| O(1) | 0.022 (3) | 0.030 (3) | 0.032 (3) | 0.007 (2) | 0.004 (2) | 0.007 (2) |
| O(2) | 0.029 (3) | 0.025 (2) | 0.044 (3) | 0.005 (2) | 0.009 (2) | 0.007 (2) |
| O(3) | 0.034 (3) | 0.022 (2) | 0.017 (2) | 0.008 (2) | −0.008 (2) | −0.005 (2) |
| O(4) | 0.029 (3) | 0.025 (2) | 0.030 (2) | 0.007 (2) | −0.004 (2) | −0.006 (2) |
| O(5) | 0.028 (2) | 0.027 (2) | 0.020 (2) | −0.008 (2) | 0.001 (2) | −0.010 (2) |
| O(6) | 0.030 (2) | 0.016 (2) | 0.023 (2) | 0.002 (2) | −0.005 (2) | −0.001 (2) |
| O(7) | 0.032 (3) | 0.027 (3) | 0.038 (3) | 0.009 (2) | −0.008 (2) | −0.018 (2) |
| O(8) | 0.023 (3) | 0.033 (3) | 0.033 (3) | 0.005 (2) | −0.002 (2) | −0.008 (2) |
| C(1) | 0.023 (3) | 0.024 (3) | 0.017 (3) | −0.007 (3) | 0.000 (2) | −0.001 (3) |
| C(2) | 0.027 (3) | 0.016 (3) | 0.020 (3) | 0.000 (3) | 0.000 (2) | −0.008 (2) |
| C(3) | 0.032 (4) | 0.042 (4) | 0.035 (4) | −0.012 (3) | 0.009 (3) | −0.013 (3) |
| C(4) | 0.040 (4) | 0.015 (3) | 0.032 (4) | 0.004 (3) | −0.001 (3) | −0.004 (3) |
| C(5) | 0.022 (3) | 0.019 (3) | 0.020 (3) | 0.009 (3) | 0.001 (2) | 0.002 (3) |
| C(6) | 0.021 (3) | 0.018 (3) | 0.022 (3) | 0.013 (3) | −0.003 (2) | 0.003 (3) |
| C(7) | 0.035 (4) | 0.036 (4) | 0.048 (5) | −0.015 (3) | 0.017 (4) | −0.005 (3) |
| C(8) | 0.035 (4) | 0.035 (4) | 0.040 (4) | 0.014 (3) | −0.012 (4) | −0.004 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| U(1)—O(1) | 1.783 (5) | C(2)—C(4) | 1.514 (9) |
| U(1)—O(2) | 1.762 (6) | C(3)—H(1) | 0.960 |
| U(1)—O(3) | 2.444 (5) | C(3)—H(2) | 0.960 |
| U(1)—O(4) | 2.407 (5) | C(3)—H(3) | 0.960 |
| U(1)—O(5)ⁱ | 2.355 (4) | C(4)—H(4) | 0.960 |
| U(1)—O(7) | 2.346 (5) | C(4)—H(5) | 0.960 |
| U(1)—O(8) | 2.336 (5) | C(4)—H(6) | 0.960 |
| O(3)—C(2) | 1.449 (8) | C(5)—C(6) | 1.525 (10) |
| O(3)—H(13) | 0.820 | C(6)—C(7) | 1.53 (1) |
| O(4)—C(1) | 1.241 (8) | C(6)—C(8) | 1.523 (10) |
| O(5)—C(1) | 1.280 (8) | C(7)—H(7) | 0.960 |
| O(6)—C(6) | 1.441 (8) | C(7)—H(8) | 0.960 |
| O(6)—H(14) | 0.820 | C(7)—H(9) | 0.960 |
| O(7)—C(5)ⁱⁱ | 1.257 (8) | C(8)—H(10) | 0.960 |
| O(8)—C(5) | 1.259 (8) | C(8)—H(11) | 0.960 |
| C(1)—C(2) | 1.528 (8) | C(8)—H(12) | 0.960 |
| C(2)—C(3) | 1.51 (1) | | |

| | | | |
|---|---|---|---|
| O(1)—U(1)—O(2) | 178.3 (2) | C(1)—C(2)—C(4) | 111.6 (6) |
| O(1)—U(1)—O(3) | 88.9 (2) | C(3)—C(2)—C(4) | 112.9 (6) |
| O(1)—U(1)—O(4) | 89.9 (2) | C(2)—C(3)—H(1) | 109.5 |
| O(1)—U(1)—O(5)ⁱ | 88.5 (2) | C(2)—C(3)—H(2) | 109.5 |
| O(1)—U(1)—O(7) | 89.5 (2) | C(2)—C(3)—H(3) | 109.5 |
| O(1)—U(1)—O(8) | 88.5 (2) | H(1)—C(3)—H(2) | 109.5 |
| O(2)—U(1)—O(3) | 89.4 (2) | H(1)—C(3)—H(3) | 109.5 |
| O(2)—U(1)—O(4) | 89.7 (2) | H(2)—C(3)—H(3) | 109.5 |
| O(2)—U(1)—O(5)ⁱ | 93.0 (2) | C(2)—C(4)—H(4) | 109.5 |
| O(2)—U(1)—O(7) | 91.7 (2) | C(2)—C(4)—H(5) | 109.5 |
| O(2)—U(1)—O(8) | 90.6 (2) | C(2)—C(4)—H(6) | 109.5 |
| O(3)—U(1)—O(4) | 62.1 (1) | H(4)—C(4)—H(5) | 109.5 |
| O(3)—U(1)—O(5)ⁱ | 135.7 (2) | H(4)—C(4)—H(6) | 109.5 |
| O(3)—U(1)—O(7) | 148.9 (2) | H(5)—C(4)—H(6) | 109.5 |
| O(3)—U(1)—O(8) | 68.9 (2) | O(7)ⁱⁱ—C(5)—O(8) | 124.4 (6) |
| O(4)—U(1)—O(5)ⁱ | 73.7 (2) | O(7)ⁱⁱ—C(5)—C(6) | 116.7 (6) |
| O(4)—U(1)—O(7) | 149.0 (2) | O(8)—C(5)—C(6) | 119.0 (6) |
| O(4)—U(1)—O(8) | 131.0 (2) | O(6)—C(6)—C(5) | 111.4 (5) |
| O(5)ⁱ—U(1)—O(7) | 75.3 (2) | O(6)—C(6)—C(7) | 105.3 (5) |
| O(5)ⁱ—U(1)—O(8) | 155.1 (2) | O(6)—C(6)—C(8) | 109.8 (6) |
| O(7)—U(1)—O(8) | 80.0 (2) | C(5)—C(6)—C(7) | 106.3 (6) |
| U(1)—O(3)—C(2) | 124.2 (3) | C(5)—C(6)—C(8) | 111.5 (6) |
| U(1)—O(3)—H(13) | 126.3 | C(7)—C(6)—C(8) | 112.2 (6) |
| C(2)—O(3)—H(13) | 109.5 | C(6)—C(7)—H(7) | 109.5 |
| U(1)—O(4)—C(1) | 126.5 (4) | C(6)—C(7)—H(8) | 109.5 |
| U(1)ⁱⁱⁱ—O(5)—C(1) | 136.7 (4) | C(6)—C(7)—H(9) | 109.5 |
| C(6)—O(6)—H(14) | 109.5 | H(7)—C(7)—H(8) | 109.5 |
| U(1)—O(7)—C(5)ⁱⁱ | 154.9 (4) | H(7)—C(7)—H(9) | 109.5 |
| U(1)—O(8)—C(5) | 153.0 (5) | H(8)—C(7)—H(9) | 109.5 |
| O(4)—C(1)—O(5) | 125.3 (6) | C(6)—C(8)—H(10) | 109.5 |
| O(4)—C(1)—C(2) | 119.3 (5) | C(6)—C(8)—H(11) | 109.5 |
| O(5)—C(1)—C(2) | 115.4 (6) | C(6)—C(8)—H(12) | 109.5 |
| O(3)—C(2)—C(1) | 102.7 (5) | H(10)—C(8)—H(11) | 109.5 |
| O(3)—C(2)—C(3) | 109.9 (5) | H(10)—C(8)—H(12) | 109.5 |
| O(3)—C(2)—C(4) | 109.3 (5) | H(11)—C(8)—H(12) | 109.5 |
| C(1)—C(2)—C(3) | 109.9 (5) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O(3)—H(13)···O(6) | 0.820 | 1.927 | 2.597 (6) | 138.188 |
| O(6)—H(14)···O(1)ⁱᵛ | 0.820 | 1.999 | 2.777 (6) | 158.201 |

Symmetry code: (iv) −*x*+1, −*y*+1, −*z*+1.