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A novel uranium-containing coordination polymer: poly[dioxouranium(VI)-μ_4-*n*-pentane-1,5-dicarboxylato]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.027
wR factor = 0.062
Data-to-parameter ratio = 16.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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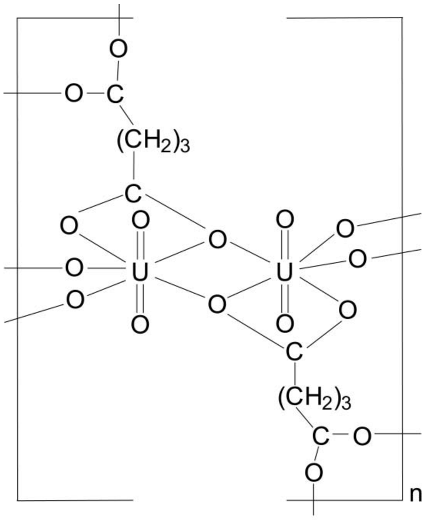
The title compound, $[U(C_5H_6O_4)O_2]$, consists of $(UO_2)_2O_8$ dimers connected by *n*-pentane-1,5-dicarboxylate (glutaric acid) molecules to form chains running in the [010] direction. These chains are further connected by the carboxylate ligand to form sheets in the $(10\overline{2})$ plane.

Comment

The title compound, (I), was synthesized during an ongoing effort to create novel metal organic framework materials containing $[UO_2]^{2+}$ centers. The structure consists of $\{(UO_2)_2O_8\}$ dimers that have previously been seen in only one compound, *viz*. $UO_2(C_6H_8O_4)$ (Borkowski & Cahill, 2003). The dimers are constructed of two edge-shared pentagonal bipyramids that consist of a central UO_2^{2+} ion surrounded by five equatorial O atoms that are from four distinct glutarate anions. The UO_2^{2+} ion contains the crystallographically unique uranium atom bonded to O1 and O2 (also called the 'uranyl' O atoms). The uranyl O atoms are found at an average distance of 1.746 (5) Å from the uranium center. The dimers are connected by bridging glutarate anions to form chains running along the [010] direction. These chains are further connected by the glutarate ligands to form two-dimensional sheets.



(I)

The dianionic carboxylate ligand has two modes of connectivity with the UO_2^{2+} cation. At one end of the ligand (O3 and O4), the O atoms form a bridging tridentate mode of connectivity, whereas at the other end (O5 and O6) they bridge the dimers into chains. Atom O3 and its symmetry equivalent are shared by two U atoms to form the shared edge of the dimer and are at a longer distance from the U atom than the rest of the equatorial O atoms [average distances of 2.469 (4) and 2.360 (4) Å, respectively].

Experimental

Uranium oxynitrate hexahydrate and glutaric acid are available commercially and were used without any further purification. Uranium oxynitrate hexahydrate (0.251 g) and glutaric acid (0.066 g) were dissolved in water (1.36 g) in the presence of concentrated aqueous ammonia (80 µl, 14 *N*). The solution (pH 3.22) was prepared in a 23 ml Teflon-lined Parr bomb then heated statically at 453 K for 3 d. Yellow crystals formed *in situ* and are insoluble in water, ethanol and acetone. Phase purity was confirmed by comparison of the observed and calculated powder X-ray diffraction patterns (*JADE*; Materials Data, 2003).

Crystal data

$[U(C_5H_6O_4)O_2]$
$M_r = 400.13$
Monoclinic, $P2_1/c$
$a = 6.0458$ (3) Å
$b = 9.3592$ (5) Å
$c = 14.0314$ (6) Å
$\beta = 90.500$ (1)°
$V = 793.92$ (7) Å^3
$Z = 4$

$D_x = 3.348$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2700 reflections
$\theta = 2.6$–27.5°
$\mu = 20.43$ mm^{-1}
$T = 298$ (2) K
Plate, yellow
0.12 × 0.11 × 0.02 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{\min} = 0.099$, $T_{\max} = 0.665$
6142 measured reflections

1785 independent reflections
1571 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.035$
$\theta_{\max} = 27.5°$
$h = -7 \rightarrow 6$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.062$
$S = 1.06$
1785 reflections
109 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 0.2377P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.95$ e Å^{-3}
$\Delta\rho_{\min} = -1.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

U1—O1	1.743 (5)	U1—O4	2.461 (4)
U1—O2	1.749 (5)	U1—O5	2.284 (4)
U1—O3	2.526 (4)	U1—O6	2.336 (4)
U1—O3$^{\rm i}$	2.414 (4)		
O1—U1—O2	178.2 (2)	U1$^{\rm i}$—O3—U1	114.91 (13)
O3$^{\rm i}$—U1—O3	65.09 (13)		

Symmetry code: (i) $2 - x, -y, 1 - z$.

H atoms on the ligand were placed in calculated positions. The C—H bond distances were fixed at 0.97 Å and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The maximum residual electron density can be found within 0.83 Å of the uranium center. The deepest hole can be found 1.20 Å from the uranium center. The crystal remained stable throughout the data collection.

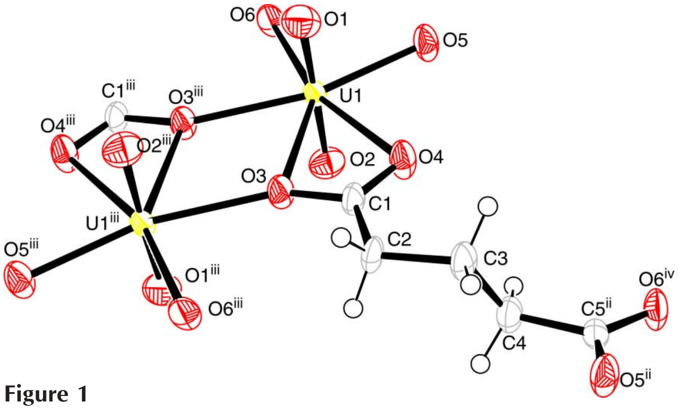


Figure 1
The asymmetric unit of the title compound, together with symmetry-equivalent atoms to complete the coordination sphere of the uranium dimer. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (ii) $-x, y + \frac{1}{2}2, -z + \frac{1}{2}$; (iii) $-x, -y, -z$; (iv) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.]

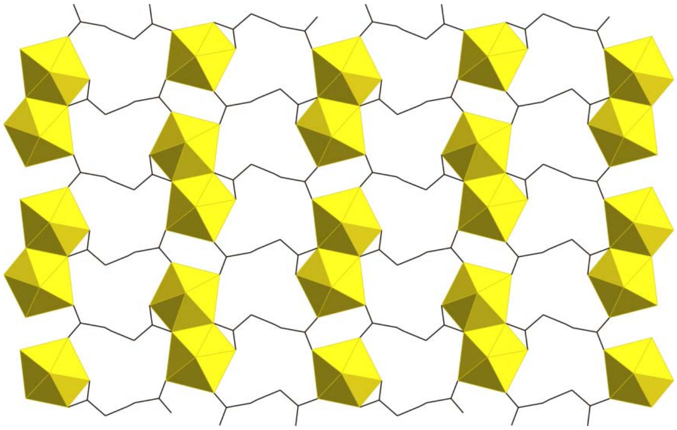


Figure 2
A single layer $(10\overline{2})$ of the title compound. Yellow polyhedra denote UO_7 coordination, black lines represent C atoms and grey spheres represent H atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalMaker* (*CrystalMaker*, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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