

Jian-Fu Xu, Ping Chen, Rubin
Zhuang, Chang-Cang Huang*
and Han-Hui ZhangDepartment of Chemistry, Fuzhou University,
Fuzhou 350002, People's Republic of China

Correspondence e-mail: cchuang@fzu.edu.cn

Key indicators

Single-crystal X-ray study

 $T = 298\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.011\text{ \AA}$ R factor = 0.025 wR factor = 0.078

Data-to-parameter ratio = 15.9

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[1,2-ethylenediammonium
[[nitratouranyl]- μ_3 -phosphito] dihydrate]**

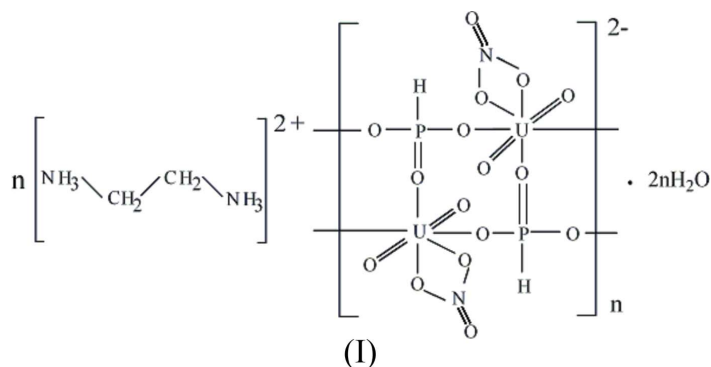
The crystal structure of the title compound, $\{(\text{C}_2\text{H}_{10}\text{N}_2)[\text{U}(\text{HPO}_3)(\text{NO}_3)\text{O}_2] \cdot 2\text{H}_2\text{O}\}_n$, consists of polymeric uranyl complex anions, ethylenediammonium cations and uncoordinated water molecules. The polymeric uranyl complex anion displays a ladder-like structure, each UO_2 unit being coordinated by three phosphite dianions and one nitrate anion with a pentagonal-bipyramidal geometry. The ethylenediammonium cation is located on an inversion center and is hydrogen bonded with the uranyl complex.

Received 14 February 2006

Accepted 7 March 2006

Comment

Many uranyl phosphates have been reported because of their applications in fields such as ion exchange and protonic conduction (Morosin, 1978). However, only four uranyl phosphites have been reported in the Cambridge Structural Database (Allen, 2002; update of November 2005). We report here the structure of the title polymeric uranyl complex, (I), which is bridged by the phosphite dianion.



The crystal structure of (I) consists of polymeric uranyl complex anions, ethylenediammonium counter-cations and uncoordinated water molecules. The polymeric uranyl complex displays a ladder-like structure (Fig. 1). Each UO_2 unit is coordinated by three phosphite dianions and one nitrate anion and has a pentagonal-bipyramidal coordination geometry. The nitrate anion chelates the U^{VI} atom with longer $\text{U}-\text{O}$ bond distances (Table 1). Each phosphite dianion bridges three UO_2 units, forming the polymeric complex chain. This is structurally similar to uranyl sulfate (Doran *et al.*, 2003) and uranyl selenate (Krivovichev & Kahlenberg, 2005).

The ethylenediammonium cation is located on an inversion center and is hydrogen bonded with the uranyl complex. The hydrogen bonds (Table 2) between the uncoordinated water molecule and the complex, and between the uncoordinated water and ethylenediammonium stabilize the crystal structure.

Experimental

UO₂(NO₃)₂·6H₂O (0.086 g, 0.17 mmol), H₃PO₃ (0.077 g, 0.94 mmol) and 1,2-ethylenediamine (0.041 g, 0.68 mmol) were mixed with distilled water (2 ml). The mixture was stirred at room temperature until completely homogenized. The solution was poured on to a watch glass and left to evaporate. Single crystals of (I) were obtained the next day.

Crystal data

(C₂H₁₀N₂)[U(HPO₃)(NO₃)O₂]-2H₂O
M_r = 922.18
 Triclinic, *P* $\bar{1}$
a = 7.0106 (17) Å
b = 7.643 (2) Å
c = 9.846 (1) Å
 α = 108.522 (7)°
 β = 100.469 (8)°
 γ = 102.125 (9)°
V = 471.20 (18) Å³
Z = 1
D_x = 3.250 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 3075 reflections
 θ = 2.3–27.5°
 μ = 17.43 mm⁻¹
T = 298 (2) K
 Needle, yellow
 0.58 × 0.17 × 0.06 mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.040, *T_{max}* = 0.342
 3928 measured reflections
 2086 independent reflections
 1949 reflections with *I* > 2σ(*I*)
R_{int} = 0.038
 θ_{max} = 27.5°
h = -9 → 8
k = -9 → 9
l = -12 → 11

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.025
wR(*F*²) = 0.078
S = 1.17
 2086 reflections
 131 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.6522P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.002$
 $\Delta\rho_{max} = 1.53 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{min} = -1.31 \text{ e } \text{Å}^{-3}$

Table 1 Selected bond lengths (Å).

U1—O1	1.784 (5)	U1—O5 ⁱⁱ	2.307 (5)
U1—O2	1.772 (6)	U1—O6	2.534 (6)
U1—O3	2.313 (5)	U1—O7	2.526 (5)
U1—O4 ⁱ	2.298 (5)		

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

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

<i>D</i> — <i>H</i> ··· <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> — <i>H</i> ··· <i>A</i>
N2—H2A···OW1 ⁱⁱⁱ	0.91	2.22	2.955 (10)	138
N2—H2A···OW1 ^{iv}	0.91	2.30	2.893 (10)	123
N2—H2B···O6 ⁱⁱ	0.91	2.33	3.104 (10)	143
N2—H2C···O3 ^v	0.91	2.49	3.136 (9)	128
N2—H2C···O5 ^v	0.91	2.10	2.975 (9)	161
OW1—H1W···O4 ^{vi}	0.82	2.37	3.142 (9)	157
OW1—H2W···O2 ^{vi}	0.82	2.31	3.080 (9)	156

Symmetry codes: (ii) *x* + 1, *y*, *z*; (iii) *x*, *y* + 1, *z*; (iv) -*x* + 2, -*y* + 2, -*z* + 1; (v) -*x* + 1, -*y* + 2, -*z* + 1; (vi) *x* + 1, *y*, *z* + 1.

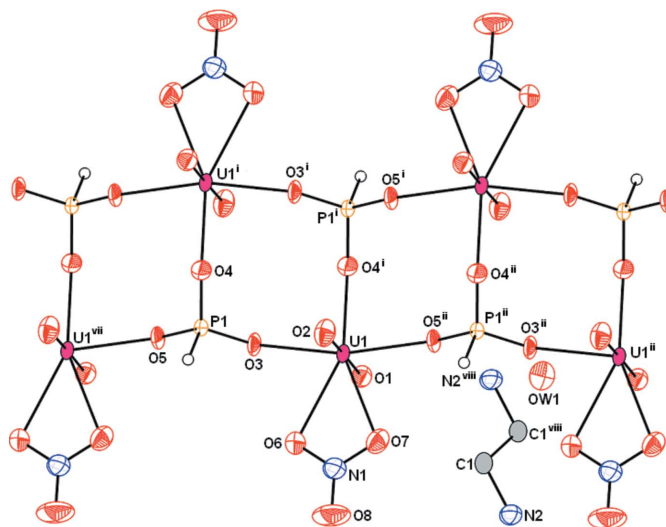


Figure 1

The molecular structure of (I), shown with 50% probability displacement ellipsoids. H atoms on the cation and on the uncoordinated water molecule have been omitted for clarity. [Symmetry codes: (i) -*x*, -*y* + 1, -*z*; (ii) *x* + 1, *y*, *z*; (vii) *x* - 1, *y*, *z*; (viii) -*x* + 2, -*y* + 2, -*z* + 1.]

H atoms on the water molecule and phosphite dianion were located in a difference Fourier map and refined as riding in their as-found relative positions, with *U_{iso}*(H) = 1.2*U_{eq}*(O,P). Methyl H atoms were placed in calculated positions, and the torsion angles refined to fit the electron density, with *U_{iso}*(H) = 1.5*U_{eq}*(C). Methylene H atoms were placed in calculated positions and refined as riding, with *U_{iso}*(H) = 1.2*U_{eq}*(C). The highest peak is 0.87 Å from atom U1 and the deepest hole is 1.27 Å from atom O5.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

The work was supported by the SRTP program of Fuzhou University and the National Natural Science Foundation of China (Nos. 20431010 and 20171012). We thank Mr Lin Yun for his assistance with data collection.

References

Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
 Doran, M. B., Norquist, A. J. & O'Hare, D. (2003). *Acta Cryst.* **E59**, m373–m375.
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
 Krivovichev, S. V. & Kahlenberg, V. (2005). *Z. Anorg. Allg. Chem.* **631**, 2352–2357.
 Morosin, B. (1978). *Acta Cryst.* **B34**, 3732–3734.
 Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
 Rigaku/MSK (2002). *CrystalStructure*. Version 3.00. Rigaku/MSK, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
 Sheldrick, G. M. (2001). *SHELXTL*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.