## metal-organic papers

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#### **Key indicators**

Single-crystal X-ray study T = 293 KMean  $\sigma(\text{N-C}) = 0.010 \text{ Å}$  R factor = 0.029 wR factor = 0.070 Data-to-parameter ratio = 19.0

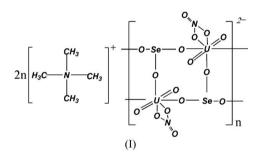
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

# Poly[tetramethylammonium [nitratouranyl- $\mu_3$ -selenito]]

The title compound,  $(C_4H_{12}N)[UO_2(NO_3)(SeO_3)]$ , consists of uranyl complex anions and  $[NMe_4]^+$  cations. Both cations and anions display mirror symmetry. Each UO<sub>2</sub> unit is coordinated by three selenite dianions and one nitrate anion with a pentagonal-bipyramidal geometry, forming anionic ladderlike chains with charge-compensating  $[NMe_4]^+$  cations intercalated between the chains.

#### Comment

Many compounds containing the uranyl ion associated with inorganic oxo-anions such as molybdate, tungstate, vanadate and phosphate have been reported because of their applications in fields of high environmental relevance (Morosin, 1978). However, only four uranyl selenites containing organic groups are included in the Cambridge Structure Database (CSD; Version 5.27; Allen, 2002). We report here the structure of the title polymeric uranyl complex, (I), bridged by selenite anions.



consists of polymeric Compound (I) uranyl  $[(UO_2)(NO_3)(SeO_3)]_n^-$  complex anions and  $[NMe_4]_n^+$ counter-cations. Both cations and anions have mirror symmetry. The polymeric uranyl complex displays a ladderlike structure as shown in Fig. 1. Each UO<sub>2</sub> unit is coordinated by three selenite dianions and one nitrate anion with a pentagonal bipyramidal coordination geometry. The nitrate chelates the U<sup>VI</sup> atom with longer U-O bond distances (Table 1). Each selenite dianion bridges three UO<sub>2</sub> units, forming a polymeric complex chain, which is structurally similar to those found in uranyl sulfate (Doran et al., 2003), uranyl selenate (Krivovichev & Kahlenberg, 2005) and uranyl phosphite (Xu *et al.* 2006). The  $[NMe_4]_n^+$  cations intercalate between the inorganic chains.

#### Experimental

© 2006 International Union of Crystallography All rights reserved A solution of  $UO_2(NO_3)_2 \cdot 6H_2O$  (0.086 g, 0.17 mmol), SeO<sub>2</sub> (0.162 g, 0.15 mmol) and [NMe<sub>4</sub>]OH (0.02 g, 0.238 mmol) in water (3 ml) was

Received 11 May 2006 Accepted 9 June 2006 stirred until completely homogenized. The mixture was poured into a small beaker and left to evaporate. Two months later, needle-like yellow–green crystals of (I) suitable for X-ray analysis had formed.

Z = 4

 $D_{\rm v} = 2.813 {\rm Mg m}^{-3}$ 

Needle, yellow-green

 $0.33 \times 0.10 \times 0.05 \text{ mm}$ 

5627 measured reflections

1669 independent reflections

1466 reflections with  $I > 2\sigma(I)$ 

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0329P)^2]$ 

 $(\Delta/\sigma)_{\rm max} < 0.001$ 

 $\Delta \rho_{\rm max} = 1.61 \text{ e } \text{\AA}^{-3}$ 

 $\Delta \rho_{\rm min} = -2.19 \text{ e} \text{ Å}^{-3}$ 

where  $P = (F_o^2 + 2F_c^2)/3$ 

Mo  $K\alpha$  radiation

 $\mu = 15.81 \text{ mm}^-$ 

T = 293 (2) K

 $R_{\rm int} = 0.051$ 

 $\theta_{\rm max} = 28.3^\circ$ 

#### Crystal data

 $(C_4H_{12}N)[U(NO_3)O_2(SeO_3)]$   $M_r = 533.15$ Monoclinic, C2/m a = 21.888 (3) Å b = 6.9501 (8) Å c = 8.3495 (10) Å  $\beta = 97.618$  (3)° V = 1259.0 (3) Å<sup>3</sup>

#### Data collection

Bruker APEXII CCD diffractometer  $\varphi$  and  $\omega$  scans Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)  $T_{\rm min} = 0.178, T_{\rm max} = 0.454$ 

#### Refinement

Refinement on  $F^2$   $R[F^2 > 2\sigma(F^2)] = 0.029$   $wR(F^2) = 0.070$  S = 1.101669 reflections 88 parameters

#### Table 1

Selected bond lengths (Å).

U1-O2	1.754 (7)	U1-O5	2.535 (4)
U1-01	1.755 (7)	Se1-O4	1.642 (5)
$U1-O4^{i}$	2.261 (5)	Se1-O3	1.669 (5)
U1-O3	2.289 (5)		

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

Methyl H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H = 0.96 Å and  $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ . The highest peak is located 1.37 Å from atom U1 and the deepest hole 0.87 Å from U1.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

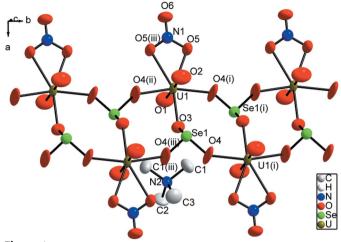


Figure 1

Part of the polymeric structure of (I), shown with 50% probability displacement ellipsoids. H atoms have been removed for clarity. [Symmetry codes: (i)  $\frac{1}{2} - x$ ,  $\frac{1}{2} - y$ , 1 - z; (ii)  $\frac{1}{2} - x$ ,  $-\frac{1}{2} + y$ , 1 - z; (iii) x, -y, z.]

*DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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