inorganic papers

Caesium zirconium uranium pentatelluride, CsZrUTe$_5$

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CsZrUTe$_5$ is isostructural with CsTiUTe$_5$. In the asymmetric unit, the site symmetries of the Cs, U, Zr, Te1, Te2 and Te3 atoms are $mm2$, $mm2$, .2/m., m.., .2. and $mm2$, respectively. CsZrUTe$_5$ has a layered structure that contains UTe$_8$ bicapped trigonal prisms sharing a common edge with ZrTe$_6$ octahedra. Cs cations separate the layers. The structure contains an infinite linear Te–Te chain, with Te atoms separated by 3.1551 (4) Å.

Comment

The structure of the compound CsTiUTe$_5$ (Cody & Ibers, 1995) features an infinite linear chain of short Te–Te interactions, the Te—Te distance being 3.065 (1) Å. Despite the presence of this chain, the compound is a semiconductor. Crystals sufficiently large to allow more complete conductivity measurements could not be grown. Accordingly, we turned our attention to the synthesis of the possible Zr analogue, namely CsZrUTe$_5$. The compound has been synthesized and its structure is reported here. Unfortunately, large crystals of this material have not been grown.
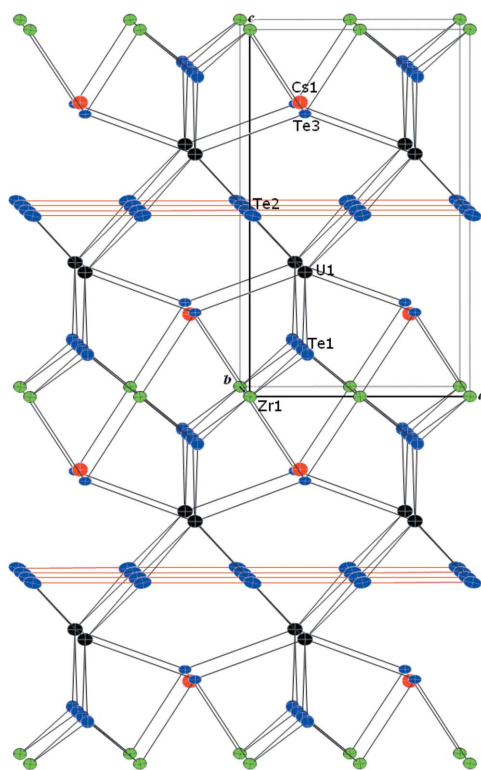
Figure 1
The structure of CsZrUTe$_5$, viewed approximately along [010]. The Te—Te bonds in the infinite chain are drawn as red lines. Displacement ellipsoids are displayed at the 99% probability level.

Fig. 1 shows the crystal structure of $CsZrUTe_5$, which is isostructural with $CsTiUTe_5$ (Cody & Ibers, 1995). The anionic layers comprise UTe_8 bicapped trigonal prisms and $ZrTe_6$ octahedra. These layers are separated by Cs cations which are coordinated in a bicapped pentagonal prism of Te atoms.

The U—Te distances and U-atom coordination environment are similar to those found in UTe_2 (Beck & Dausch, 1988). In both structures, the UTe_8 bicapped trigonal prisms have a short Te—Te distance at one edge of the triangular face. In $CsZrUTe_5$ the prisms share edges of a rectangular face through Te2 atoms in the [100] direction. This results in an infinite linear chain of Te atoms; the Te—Te distance is 3.1551 (4) Å.

Each nearly regular $ZrTe_6$ octahedron shares faces with two adjacent octahedra to create an unusual infinite $[ZrTe_3^{2-}]$ chain. The Zr—Te distances (Table 1) are comparable with those of 2.8771 (7)–3.0426 (8) Å in ZrTe (Örlygsson & Harbrecht, 2001).

Experimental

$CsZrUTe_5$ was obtained as black needles from the reaction of Cs_2Te_3 (0.11 mmol), U (Oak Ridge National Laboratory, 0.23 mmol), Zr (Chemtall GmbH, 0.23 mmol) and Te (Aldrich, 99.8%, 0.80 mmol) with CsCl (Strem, 99.999%) as flux. The Cs_2Te_3 reactive flux was prepared by the stoichiometric reaction of Cs (Alfa Aesar, 99.8%) and Te in liquid NH_3 at 194 K. The reactants were loaded into a fused-silica tube under an Ar atmosphere in a dry box. The tube was evacuated to 10^{-4} Torr (1 Torr = 133.322 Pa), sealed and placed in a computer-controlled furnace. The sample was heated to 1223 K, kept at 1223 K for 144 h and then slowly cooled at 2 K h^{-1} to 293 K. The resulting crystals were extracted manually from the melt.

Crystal data

$CsZrUTe_5$	$Z = 2$
$M_r = 1100.16$	$D_x = 6.675$ Mg m^{-3}
Orthorhombic, $Pmma$	Mo $K\alpha$ radiation
$a = 6.3101 (8)$ Å	$\mu = 31.99$ mm^{-1}
$b = 8.2299 (10)$ Å	$T = 153 (2)$ K
$c = 10.5401 (13)$ Å	Needle, black
$V = 547.36 (12)$ Å^3	$0.336 \times 0.062 \times 0.056$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	6537 measured reflections
	801 independent reflections
ω scans	769 reflections with $I > 2\sigma(I)$
Absorption correction: numerical face-indexed (*SHELXTL*; Sheldrick, 2003)	$R_{int} = 0.038$
	$\theta_{max} = 28.9°$
$T_{min} = 0.039$, $T_{max} = 0.217$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.025$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.067$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.27$	$\Delta\rho_{max} = 3.85$ e Å^{-3}
801 reflections	$\Delta\rho_{min} = -2.55$ e Å^{-3}
28 parameters	

Table 1
Selected bond lengths (Å).

U1—Te1	3.0961 (6)	Te2—Te2^{ii}	3.1551 (4)
U1—Te2	3.1118 (4)	Cs1—Te1^{iii}	3.8725 (5)
U1—Te3^i	3.3599 (4)	Cs1—Te2	3.9828 (6)
Zr1—Te3^i	2.8890 (6)	Cs1—Te1^{iv}	4.0608 (8)
Zr1—Te1	2.9087 (4)	Cs1—Te3	4.1193 (5)

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

The structure was standardized by means of the program *STRUCTURE TIDY* (Gelato & Parthé, 1987). The highest peak is 0.03 Å and the deepest hole is 1.82 Å from atom U.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 2003); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *CRYSTALMAKER* (*CRYSTALMAKER* Software, 2005); software used to prepare material for publication: *SHELXTL*.

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