Two new compounds, β-ScTe and Y₃Au₂, and a reassessment of Y₂Au

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Two new compounds, β-ScTe (scandium telluride) and Y_3Au_2 (triyttrium digold), have been synthesized by high-temperature solid-state techniques and their crystal structures, along with that of Y_2Au (diyttrium gold), have been refined by single-crystal X-ray diffraction methods. β-ScTe is a superstructure of ScTe (NiAs-type), featuring double hexagonal close-packed layers of Te atoms with the octahedral cavities filled by Sc atoms. Y_3Au_2 displays a U_3Si_2-type structure and is built from Au_2-centered bitrigonal prisms and centered cubes of Y atoms. The structure of Y_2Au is better described as an inverse $PbCl_2$-type structure rather than a Co_2Si-type.

Comment

Research within solid-state chemistry on ternary and polynary compounds has attracted much attention during the past few decades because of their interesting structures, bonding and physical properties. Knowledge of binary compounds can provide significant references during the exploratory synthesis of polynary compounds, and their identification is therefore valued. Although many binary combinations of elements are covered by binary phase diagrams and the crystal databases, some have been missed because of the limitations of the earlier experiments. For instance, only two compounds, *viz.* ScTe and Sc_2Te_3, were in the Sc–Te phase diagram reported in 1990 (Okamoto, 1990), missing several examples, Sc_2Te, Sc_8Te_3 and Sc_9Te_2, which were discovered later during the study of ternary systems (Maggard & Corbett, 1997, 1998, 2000). We discovered that the structure of β-ScTe was still missing, with an inverse Li_2O_2-type structure, a double hexagonal close-packed (dhcp) version of ScTe (NiAs-type) (Men kov *et al.*, 1961). Y_3Au_2 was missed in the investigation of the Y–Au phase diagram (Saccone *et al.*, 1997), whereas Y_2Au was identified as Co_2Si-type (Yakinthos *et al.*, 1978) from lattice parameters only; no refinement of powder diffraction intensities was carried out. The crystal structures of these three phases are described here.

β-ScTe is presumably a high-temperature phase with an inverse Li_2O_2-type structure. A view of the unit cell approximately along [001] is shown in Fig. 1(*a*) and a section
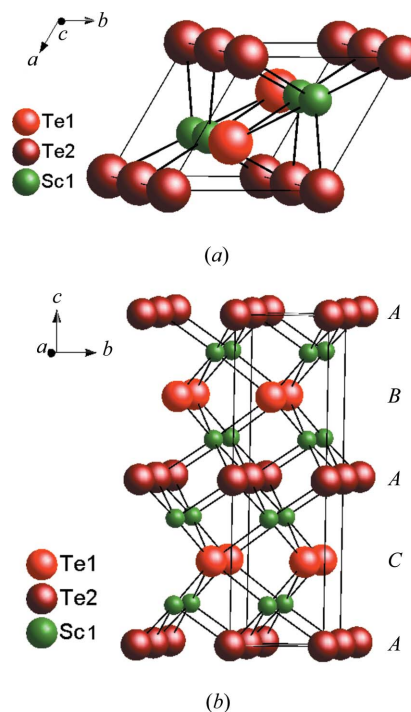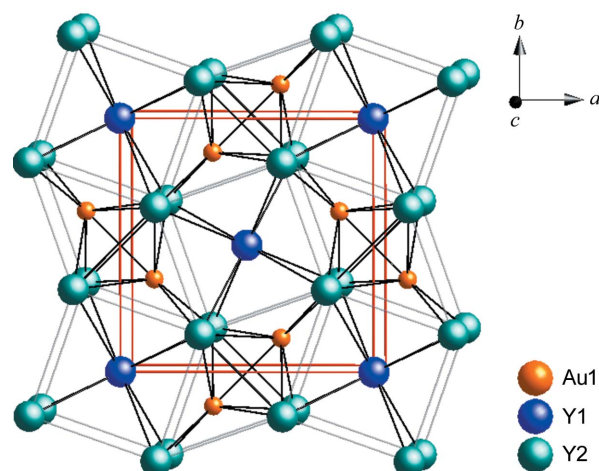

Figure 1
(*a*) A view of one unit cell, approximately along [001]. (*b*) A section of β-ScTe, approximately along [100].

approximately along [100] is shown in Fig. 1(*b*), in which Te atoms form hexagonal close-packed (hcp) layers with $ABAC\ldots$ stacking, leaving all nominal octahedral cavities filled by Sc atoms. Note that ScTe (NiAs-type) crystallizes in the same space group, $P6_3/mmc$, with $a = 4.130\,(5)$ Å and $c = 6.749\,(5)$ Å, and contains simple hcp Te atoms of $ABAB\ldots$ ordering with Sc atoms occupying the octahedral cavities (Men kov *et al.*, 1961). Therefore, β-ScTe is a stacking variant of ScTe, with a c axis twice as large.

Y_3Au_2 crystallizes in the U_3Si_2-type structure in the space group $P4/mbm$ (No. 127). An approximately [001] projection along the short 3.907 (3) Å c axis is shown in Fig. 2. The basic building units are an Au_2-centered bitrigonal prism (BTP) of

Figure 2
A projection of Y₃Au₂, approximately along [001].
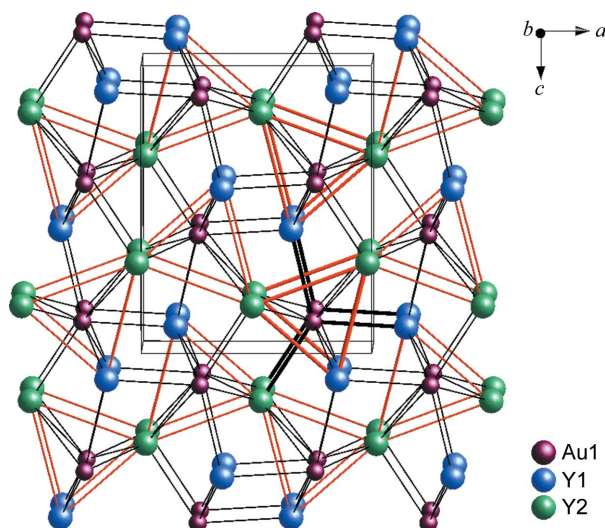
Figure 3
A view of Y_2Au, approximately along [001].

Y2 atoms and a Y1-centered Y2 cube. The Au_2 unit is an unusual dimer 3.0539 (19) Å long. The two-dimensional motif is created in such a way that each Y2 cube, with the centered Y1 atom on a fourfold axis, interconnects with four identical units through shared Y2–Y2 edges, leaving the cavities filled by the BTPs. The centered Y1 and Au1 atoms lie on a mirror plane at $c = 0$. The two-dimensional motif repeats along c to form a three-dimensional network, sharing bitriangular and square faces.

The structure of Y_2Au in the space group $Pnma$ projected along [010] is shown in Fig. 3, in which each Au atom forms the center of a trigonal prism (TP) of Y1 or Y2 atoms that shares trigonal faces with identical units to generate an infinite one-dimensional column along b. The TPs interconnect with shared Y2–Y2 edges and lead to the formation of puckered sheets along a. Adjoining sheets stack along c, with displacements of $b/2$, to create a three-dimensional structural network. As a result, each TP is tricapped by two Y1 atoms and one Y2 atom so that each Au atom has nine neighbors. Y_2Au is better described as an inverse $PbCl_2$-type structure rather than the earlier reported Co_2Si-type, in which the Si atom would have ten neighbors (Flahaut & Thévet, 1980; Liu & Corbett, 2006).

Experimental

The formation of all three phases was in fact first noted in powder pattern data from nearby ternary systems. β-ScTe was synthesized from a mixture of Sc and Sc_2Te_3. The latter was obtained from a prereaction of Sc and Te in a 2:3 ratio, sealed in a silica tube under vacuum, heated at 723 K for 12 h and then at 1173 K for 72 h. Y_3Au_2 and Y_2Au were prepared from mixtures of high-purity elements. The three combinations were each pelletized and arc-melted under an argon atmosphere in a glove-box. The pellets were then sealed in tantalum containers and annealed in a graphite-heated vacuum furnace at 1573 K for 200 h for β-ScTe, and at 1323 K for one week for Y_3Au_2 and Y_2Au. The products were crushed with the aid of an agate mortar into small crystals that were suitable for single-crystal X-ray diffraction.

ScTe

Crystal data

ScTe
$M_r = 172.56$
Hexagonal, $P6_3/mmc$
$a = 4.0969$ (6) Å
$c = 13.602$ (3) Å
$V = 197.71$ (6) Å^3

$Z = 4$
Mo $K\alpha$ radiation
$\mu = 17.64$ mm^{-1}
$T = 293$ K
$0.15 \times 0.08 \times 0.07$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.177$, $T_{max} = 0.372$

1274 measured reflections
92 independent reflections
90 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.081$
$S = 1.57$
92 reflections

8 parameters
$\Delta\rho_{max} = 1.21$ e Å^{-3}
$\Delta\rho_{min} = -1.65$ e Å^{-3}

Y_3Au_2

Crystal data

Y_3Au_2
$M_r = 660.66$
Tetragonal, $P4/mbm$
$a = 8.059$ (3) Å
$c = 3.907$ (3) Å
$V = 253.7$ (3) Å^3

$Z = 2$
Mo $K\alpha$ radiation
$\mu = 91.35$ mm^{-1}
$T = 293$ K
$0.05 \times 0.04 \times 0.02$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.092$, $T_{max} = 0.262$

1866 measured reflections
194 independent reflections
156 reflections with $I > 2\sigma(I)$
$R_{int} = 0.093$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.069$
$S = 0.93$
194 reflections

11 parameters
$\Delta\rho_{max} = 1.46$ e Å^{-3}
$\Delta\rho_{min} = -1.40$ e Å^{-3}

Y_2Au

Crystal data

Y_2Au
$M_r = 374.79$
Orthorhombic, $Pnma$
$a = 7.115$ (3) Å
$b = 4.933$ (2) Å
$c = 8.908$ (4) Å

$V = 312.7$ (2) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 83.29$ mm^{-1}
$T = 293$ K
$0.12 \times 0.08 \times 0.04$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.036$, $T_{max} = 0.135$

1619 measured reflections
345 independent reflections
299 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.058$
$S = 1.07$
345 reflections

20 parameters
$\Delta\rho_{max} = 1.76$ e Å^{-3}
$\Delta\rho_{min} = -2.14$ e Å^{-3}

For all three title compounds, data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXTL*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FN3086). Services for accessing these data are described at the back of the journal.

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