

Two new binary lanthanide polytellurides: Syntheses and crystal structures of $\text{CeTe}_{1.90}$ and $\text{SmTe}_{1.80}$

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Abstract

Single crystals of the new binaries $\text{CeTe}_{1.90}$ and $\text{SmTe}_{1.80}$ have been obtained. $\text{CeTe}_{1.90}$ was synthesized at 1023 K from the reaction of Ce, TeO_2 , and Te with the use of a CsCl flux. It crystallizes in the tetragonal space group $P4_2/n$ with 20 formula units in a cell of dimensions at 153 K of $a = 10.0261(5)$, $c = 18.1336(12)$ Å, $V = 1822.84(18)$ Å³. It is isostructural with the $\text{LnSe}_{1.9}$ polyselenides ($\text{Ln} = \text{La, Ce, Pr}$) and with $\text{SmS}_{1.90}$. $\text{SmTe}_{1.80}$ was synthesized at 1223 K from the reaction of Sm and Te in a KBr flux. $\text{SmTe}_{1.80}$ crystallizes in a new structural type in the tetragonal space group $P4/n$ with 20 formula units in a cell of dimensions at 153 K of $a = 9.7026(4)$, $c = 18.0072(14)$ Å, $V = 1695.21(14)$ Å³. Both of these layered structures, which may be derived from the ZrSiS structure type, consist of double layers of $[\text{LnTe}]$ polyhedra separated by planar Te nets that contain vacancies. In these nets the shortest Te–Te distances are 2.9194(5), 3.1204(5), and 3.3324(6) Å in $\text{CeTe}_{1.90}$ and 2.878(1), 2.9932(3), and 3.2114(7) Å in $\text{SmTe}_{1.80}$. Neither a simple delineation of the Te–Te bonding nor an assignment of individual formal oxidation states is possible in either of these compounds if one takes strict account of the Te–Te distances.

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1. Introduction

The binary lanthanide polychalcogenides LnQ_2 and their LnQ_{2-x} derivatives ($\text{Ln} = \text{lanthanide}$, $Q = \text{S, Se, Te}$) have been extensively studied, especially for $Q = \text{S}$ [1], because of their interesting physical properties and rich structural chemistry. Physical properties include thermodynamic, magnetic, optical, transport, thermoelectric, and charge density wave behavior [2–14]. The structural features of many of these compounds have been reviewed [1,15]. These layered phases, which may be derived from the ZrSiS structure type and also may be considered as superstructures of the anti- Cu_2Sb structure type, consist of double layers of $[\text{LnQ}]$ polyhedra separated by planar Q nets [15–19]. The hypostoichiometry common in these compounds arises entirely from vacancies in these planar nets. In some structures these vacancies are ordered [16,17,19] whereas in others they are not [11,13]. Theore-

tical calculations have attempted to rationalize the distortions of these nets and the resultant superstructures [20–22].

Among the X-ray single-crystal studies of Ce/Te and Sm/Te phases that have been carried out are those for CeTe_2 [13,23], SmTe_3 [6], $\text{SmTe}_{1.84}$ [11], and Sm_2Te_5 [6]. The present paper describes the syntheses and the crystal structures of the two new binary polytellurides $\text{CeTe}_{1.90}$ and $\text{SmTe}_{1.80}$.

2. Experimental

2.1. Syntheses

2.1.1. $\text{CeTe}_{1.90}$

Black block-shaped single crystals of $\text{CeTe}_{1.90}$ were obtained in the reaction of Ce (20 mmol, Alfa, 99.9%), TeO_2 (1 mmol), and Te (27 mmol, Aldrich, 99.8%). TeO_2 was synthesized by dissolving Te metal in aqua regia at 353 K, followed by the slow addition of NH_4OH . The resultant precipitate of TeO_2 was filtered and washed with

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deionized water. Its purity was established by means of an X-ray powder diffraction pattern. A CsCl (Strem, 99.9%) flux in approximately five times molar excess was used to promote the growth of single crystals. The starting materials were mixed together in a fused-silica tube that was then evacuated to approximately 10^{-5} Torr and sealed. The tube was heated to 1023 K over 48 h, kept at 1023 K for 5 days, cooled at 1.5 K/h to 873 K, and then the furnace was turned off. The reaction mixture was washed free of chloride salts with water and then dried with acetone. The yield of $\text{CeTe}_{1.90}$ was about 5%.

2.1.2. $\text{SmTe}_{1.80}$

Sm (1 mmol, Alfa, 99.9%), Te (2 mmol, Aldrich, 99.8%), and KBr (4 mmol, Alfa, 99%) were mixed together and loaded into a fused-silica tube in an argon-filled dry box. The tube was then evacuated to approximately 10^{-5} Torr, sealed, and placed in a furnace. The tube was heated to 1223 K over 72 h, kept at 1223 K for 4 days, cooled at 2.5 K/h to 973 K, and then the furnace was turned off. The reaction mixture was washed free of bromide salts with water and then dried with acetone. Black block-shaped crystals of $\text{SmTe}_{1.80}$ suitable for X-ray structure analysis were produced in about 5% yield.

Semiquantitative analyses performed with a Hitachi 3500N SEM confirmed the presence of Ce or Sm and Te in the approximate ratio of 1:2, in reasonable agreement with the X-ray structure determinations from which the stated formulas were derived. The SEM studies provided no evidence for the presence of other heavier elements or of O in either compound. Both compounds are modestly stable in air.

2.2. Crystallography

For each compound a single crystal was placed in the cold stream of a Bruker SMART-1000 CCD diffractometer [24]. The crystal was kept at 153 K throughout the data collection. X-ray diffraction data were collected with the use of monochromatized $\text{MoK}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). The diffracted intensities generated by a scan of 0.3° in ω were recorded on sets of 606 frames at ϕ angles of 0° , 90° , 180° , and 270° with the use of the program SMART [24]. The exposure time was 15 s per frame. The resultant frames were free of obvious diffuse scattering. Because both super cells and twinning are known to occur in some of the rare-earth hypochalcogenides [19,25] additional exposures of 30 s/frame were employed in the collection of three groups of frames. For each compound reflections in diverse regions of reciprocal space on both the 30- and 15-s frames were centered with the use of the program SMART [24]. A low threshold value of 5.0 for $I/\sigma(I)$ was employed. Because possible superlattice reflections might have very low intensities [25] the stronger reflections were deleted to ensure that a large number of weak reflections remained. The program CELL_NOW [26] was used to obtain possible unit cells and twinning conditions. In each instance, it

provided the unit cell reported here and it gave no evidence for supercells or for twinning. For each compound data reduction and the final cell refinement were carried out with the use of the program SAINT [24] and face-indexed absorption corrections were carried out numerically with the program XPREP [27]. Then the program SADABS [27] was employed to make incident beam and decay corrections.

Each structure was solved with the direct methods program SHELXS and refined with the full-matrix least-squares program SHELXL of the SHELXTL suite of programs [27]. The refinement of the Ce structure in the centrosymmetric space group $P4_2/n$ was straightforward and resulted in satisfactory anisotropic displacement parameters for all atoms. The resultant values of R and R_w are 0.032 and 0.085, respectively. Each atomic site is fully occupied; the final composition from the X-ray structure determination is $\text{CeTe}_{1.90}$. This space group and the resultant structure are known for the $\text{LnSe}_{1.9}$ polyselenides ($\text{Ln} = \text{La, Ce, Pr}$) [16,17], $\text{SmS}_{1.90}$ [19], and $\text{SmTe}_{1.84}$ [11]. As opposed to $\text{CeTe}_{1.90}$, $\text{SmTe}_{1.80}$ does not crystallize in space group $P4_2/n$ but rather in space group $P4/n$. (There are 45 out of 51 exceptions to the systematic absences for 00ℓ reflections required in the former space group.) Solution and refinement of the $\text{SmTe}_{1.80}$ structure were straightforward in the latter space group. The resultant equivalent isotropic displacement parameter for atom Te(3) was excessively large. Anisotropic refinement, including the occupancy of atom Te(3), refined satisfactorily to values of R and R_w of 0.025 and 0.064, respectively, and to a value for the occupancy of atom Te(3) of 0.497(1). The occupancy was fixed at 0.5 in the final refinement. The resultant composition is $\text{SmTe}_{1.80}$. Despite the excellent refinement, concern over the disorder of atom Te(3) led us to attempt to re-solve the structure in several lower symmetry space groups, including $Pm\bar{m}n$, $P2/n$, $P2/c$, and $P\bar{1}$. These attempts were unsuccessful. Subsequently,

Table 1
Crystal data and structure refinement for $\text{CeTe}_{1.90}$ and $\text{SmTe}_{1.80}$

	$\text{CeTe}_{1.90}$	$\text{SmTe}_{1.80}$
Formula weight	382.56	380.03
Space group	$P4_2/n$	$P4/n$
a (Å)	10.0261(5)	9.7026(4)
c (Å)	18.1336(12)	18.0072(10)
Volume (Å ³)	1822.84(18)	1695.21(14)
Z	20	20
T (K)	153	153
λ (MoK α) (Å)	0.71073	0.71073
ρ_c (g/cm ³)	6.970	7.445
μ (cm ⁻¹)	271.05	321.94
Transmission factors	0.072–0.205	0.030–0.164
Total reflections/unique reflections	21946/2322	20458/2152
$R(F)^a$ ($F_o^2 > 2\sigma(F_o^2)$)	0.032	0.025
$R_w(F_o^2)^b$ (all data)	0.085	0.064

$$^a R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$$

$$^b R_w(F_o^2) = [\sum w(F_o^2 - F_c^2)^2 / \sum w F_o^4]^{1/2}, \quad w^{-1} = \sigma^2(F_o^2) + (0.025 \times F_o^2)^2 \quad \text{for } F_o^2 > 0; \quad w^{-1} = \sigma^2(F_o^2) \quad \text{for } F_o^2 \leq 0.$$

Table 2
Selected bond lengths (Å) for CeTe_{1.90} and SmTe_{1.80}

CeTe _{1.90}		SmTe _{1.80}	
Ce(1)–Te(5)	3.2597(4)	Sm(1)–Te(3) ^a	3.1142(6)
Ce(1)–Te(6)	3.3046(4)	Sm(1)–Te(4)	3.1378(4)
Ce(1)–Te(3)	3.3106(5)	Sm(1)–Te(1)	3.1633(4)
Ce(1)–Te(2)	3.3130(6)	Sm(1)–Te(4)	3.1967(4)
Ce(1)–Te(1)	3.3136(5)	Sm(1)–Te(4)	3.2071(4)
Ce(1)–Te(2)	3.3170(5)	Sm(1)–Te(7)	3.2345(3)
Ce(1)–Te(3)	3.3282(5)	Sm(1)–Te(4)	3.2363(5)
Ce(1)–Te(1)	3.3866(5)	Sm(1)–Te(5)	3.3036(4)
Ce(1)–Te(4)	3.4183(5)	Sm(1)–Te(3)	3.4044(6)
Ce(2)–Te(3)	3.2368(5)	Sm(2)–Te(1)	3.1578(4)
Ce(2)–Te(2)	3.2418(4)	Sm(2)–Te(6)	3.1799(3)
Ce(2)–Te(3)	3.2504(4)	Sm(2)–Te(5)	3.1997(4)
Ce(2)–Te(4)	3.2623(5)	Sm(2)–Te(2)	3.2062(4) × 2
Ce(2)–Te(2)	3.2687(4)	Sm(2)–Te(2)	3.2390(4)
Ce(2)–Te(1)	3.2712(5)	Sm(2)–Te(2)	3.2629(5)
Ce(2)–Te(5)	3.2932(4)	Sm(2)–Te(1)	3.3169(4)
Ce(2)–Te(4)	3.3266(5)	Sm(3)–Te(7)	3.2546(7)
Ce(3)–Te(3)	3.2702(4) × 2	Sm(3)–Te(4)	3.2625(4) × 4
Ce(3)–Te(5)	3.2935(7)	Sm(3)–Te(1)	3.2754(5) × 4
Ce(3)–Te(1)	3.3034(5) × 2	Sm(4)–Te(2)	3.1338(3) × 4
Ce(3)–Te(2)	3.3294(4) × 2	Sm(4)–Te(3)	3.1415(7) × 4
Ce(3)–Te(4)	3.3955(5) × 2	Sm(4)–Te(6)	3.1583(7)
Te(1)–Te(4)	2.9194(5)	Te(1)–Te(5)	2.9932(3)
Te(1)–Te(4)	3.1204(5)	Te(3)–Te(3)	2.878(1)
Te(1)–Te(6)	3.3324(5)	Te(1)–Te(3)	3.2114(7)

^aThe occupancy of atom Te(3) is 0.5.

careful examination of the structure solution in space group $P4/n$ led to a rationalization for this disorder, as will be discussed below.

In both structures the program Structure Tidy [28] was used to standardize the positional parameters. Selected crystallographic data are listed in Table 1 and in Supplementary information. Selected bond distances for CeTe_{1.90} and SmTe_{1.80} are reported in Table 2.

3. Results and discussion

3.1. Syntheses

Ce, TeO₂, and Te were reacted at 1023 K in an effort to produce a cerium oxytelluride. Instead, the reaction afforded a 5% yield of high quality crystals of CeTe_{1.90}. Sm and Te together with a KBr flux were reacted at 1223 K in a successful effort to synthesize a samarium telluride. High-quality crystals of SmTe_{1.80} were obtained in about a 5% yield. No effort was made to increase the yields of either compound.

3.2. Crystal structures

The structures of the LnQ_2 compounds as well as their chalcogen-deficient LnQ_{2-x} derivatives have been discussed in detail (see, for example, [15]). These structures, which may be derived from the ZrSiS structure type (space group $P4/nmm$) [29], consist of double layers of $[LnQ]$ polyhedra

separated by essentially planar Q nets. In the LnQ_{2-x} hypostoichiometric derivative structures these nets possess vacancies, ordered or random. The LnQ_{2-x} derivatives crystallize in a number of subgroups of $P4/nmm$, mainly in the tetragonal and orthorhombic systems, depending on the nature of these vacancies and the concomitant distortions of the nets. CeTe_{1.90}, a new binary in the Ce/Te system, crystallizes in space group $P4_2/n$ and is isostructural with the $LnSe_{1.9}$ polyselenides ($Ln = La, Ce, Pr$) [16,17]. Its structure is illustrated in Fig. 1. SmTe_{1.80}, a new binary in the Sm/Te system, crystallizes in space group $P4/n$ and possesses a different defect Te net.

In the CeTe_{1.90} structure the three independent Ce atoms are coordinated by 9, 8, and 9 Te atoms, respectively. The Ce–Te distances range from 3.2368(5) to 3.4183(5) Å. The corresponding range in the structure of CeTe₂ is 3.28 to 3.33 Å [30] but see [13]. In the SmTe_{1.80} structure the four independent Sm atoms are coordinated by 9, 8, 9, and 9 Te

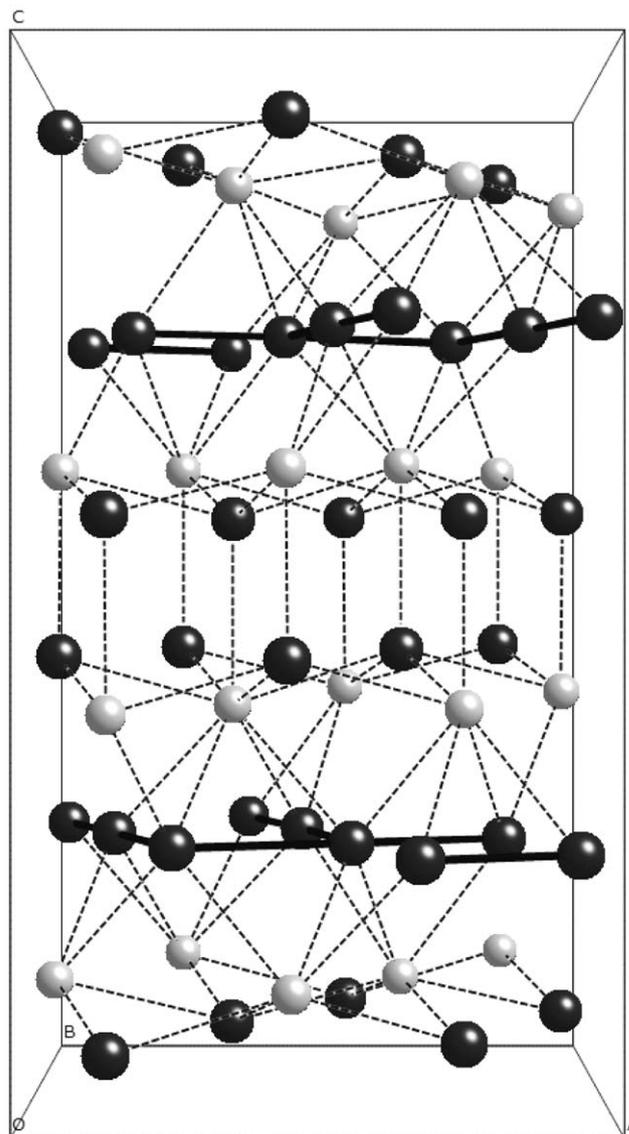


Fig. 1. View along [010] of the unit cell of CeTe_{1.90}.

atoms, respectively. The Sm–Te distances range from 3.1142(6) to 3.4044(6) Å; these may be compared with distances of 3.196(1)–3.336(1) Å in SmTe₃ [6].

Visualization of specific $[Q_n]^{m-}$ anions in binary lanthanide polychalcogenides and concomitant assignment of formal oxidation states are common. Such formulations often tend to emphasize geometries and to discount variations in $Q-Q$ distances. We prefer to take a more conservative approach by emphasizing the Te–Te distances in descriptions of the nets in the present structures. The shortest Te–Te distance in elemental Te is 2.8345(8) Å and the next shortest interaction is 3.4912(8) Å [31]. The importance of second-nearest-neighbor Te···Te interactions has been noted [22]. Accordingly, we have chosen to draw bonds for such interactions. Thus, in Fig. 2 the Te net in CeTe_{1.90} is displayed with bonds drawn for the three shortest Te···Te interactions, namely those of 2.9194(5), 3.1204(5), and 3.3324(5) Å (Table 2). The next shortest Te···Te interaction in the net is 3.595 Å. Atom Te(6) lies on a site of symmetry $\bar{4}$. The net is essentially planar; for example, the mean deviation from the least-squares plane through the 8-atom Te4/Te1 net is 0.009 Å. Despite the asymmetric nature of the 8-atom net, consisting as it does

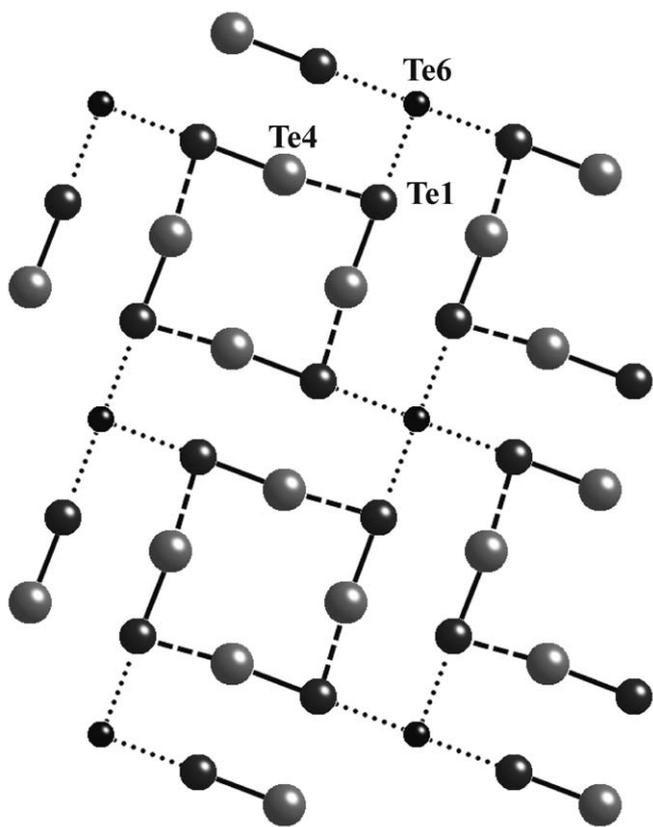


Fig. 2. The Te net near $z = 0.25$ in CeTe_{1.90}. The view is down [001]. The crystallographically independent atoms Te(1), Te(4), and Te(6) are drawn with different arbitrary radii to facilitate their identification in the net. Bonds are drawn for the three shortest Te–Te interactions, namely Te(1)–Te(4) (2.9194(5) Å (solid line) and 3.1204(5) Å (dashed line)) and Te(1)–Te(6) (3.3324 Å (dotted line)). Atom Te(6) sits on a site of symmetry $\bar{4}$.

of alternating bonds of length 2.9194(5) and 3.1204(5) Å. the net is ordered, at least in the model chosen here. If the net consisted of interacting Te₂²⁻ pairs, then atom Te(4) would be split into two half-atoms separated by about 0.4 Å. Although attempts to refine such a model were unsuccessful, the Bragg X-ray experiment affords only electron density smeared by noise from various sources. Its interpretation will always be somewhat subjective and model dependent.

Fig. 3 displays the Te net in SmTe_{1.80} with bonds drawn for the three shortest Te···Te interactions of 2.878(1), 2.9932(3), and 3.2114(7) Å (Table 2). The next shortest Te···Te interaction is 3.444 Å. In this net atom Te(5) has site symmetry 2. All atoms in this net are ordered except at the Te(3) site. The fourfold axes parallel to the c -axis and perpendicular to the nets generate sites of four half-occupied Te(3) atoms, as illustrated in Fig. 3. Because adjacent Te(3) atoms are separated by the physically impossible distance of 2.0351(8) Å only the diagonal bonds of length 2.878(1) Å can be present among these half-occupied Te(3) atoms. The resultant structure comprises two sets of Te chains. Only one of the sets can be present in a given net. The two sets occur in equal numbers throughout the structure, presumably in a random fashion because diffuse scattering was minimal and no evidence of a super cell was found. Of course, in the unit cell these two sets are superimposed; hence the half-occupancy of the Te(3) atom. The chains are nearly planar; for example, the Te3–Te3–Te1–Te5–Te1–Te3 segment has a mean deviation from the least-squares plane of 0.071 Å.

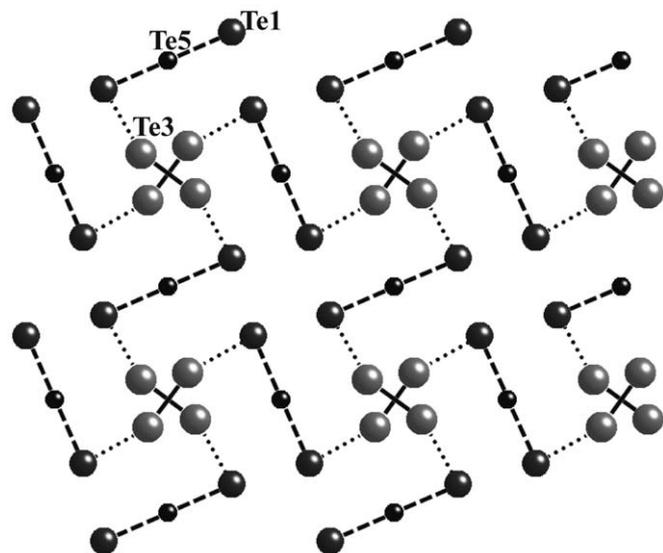


Fig. 3. The Te net near $z = 0.25$ in SmTe_{1.80}. The view is down [001]. The crystallographically independent atoms Te(1), Te(3), and Te(5) are drawn with different arbitrary radii to facilitate their identification in the net. Bonds are drawn for the three shortest Te–Te interactions, namely Te(3)–Te(3) (2.878(1) Å (solid line) across the diagonal of the disordered half atoms), Te(1)–Te(5) (2.9932(3) Å (dashed line), and Te(1)–Te(3) (3.2114(7) Å (dotted line)). The two sets of chains, equally distributed throughout the structure, are superimposed in the unit cell. Atom Te(5) sits on a site of site symmetry 2.

In the $\text{SmTe}_{1.80}$ structure described here, all atoms refined anisotropically and only the Te(3) atom position is not fully occupied. Contrast this structure with that reported for $\text{SmTe}_{1.84}$ [11]. $\text{SmTe}_{1.84}$ was described in space group $P4_2/n$ in a cell $a = 9.709(1)$, $c = 18.008(7)$ Å at 293 K that is strikingly similar to the one described here ($a = 9.7026(4)$, $c = 18.0072(10)$ Å at 153 K). In the asymmetric unit three Sm atoms and nine Te atoms were found. Of the nine Te atoms, six were not fully occupied but had occupancies that varied from 0.85 to 0.14 and three of these could not be refined anisotropically. The composition $\text{SmTe}_{1.84}$ was derived from the X-ray refinement. There is no way of knowing if $\text{SmTe}_{1.80}$ described here and $\text{SmTe}_{1.84}$ [11] are the same phase. Note, however, that in the Sm/S system three discrete phases of nearly the same stoichiometry, namely $\text{SmS}_{1.863}$, $\text{Sm}_{1.893}$, and $\text{Sm}_{1.900}$, have been identified by thermodynamic means [2]. How these phases differ structurally is not known.

Supplementary material

The crystallographic files in cif format for $\text{CeTe}_{1.90}$ and $\text{SmTe}_{1.80}$ have been deposited with FIZ Karlsruhe as CSD numbers 416368 and 416367, respectively. These data may be obtained free of charge by contacting FIZ Karlsruhe at +49 7247 808 666 (fax) or crysdata@fiz-karlsruhe.de (e-mail).

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Appendix A. Supplementary Materials

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.jssc.2006.07.010](https://doi.org/10.1016/j.jssc.2006.07.010).

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