LaTe$_{1.9}$: a tenfold superstructure of the ZrSSi type

Hagen Poddig and Thomas Doert*

Faculty of Chemistry and Food Chemistry, TU Dresden, D-01062 Dresden, Germany. *Correspondence e-mail: thomas.doert@tu-dresden.de

Single crystals of LaTe$_{1.9}$ (lanthanum telluride) have been obtained by chemical transport reactions with iodine as transport agent. LaTe$_{1.9}$ adopts the CeSe$_{1.9}$ structure type and crystallizes in the space group $P4_2/n$ with lattice parameters $a = 10.1072$ (3) Å and $c = 18.2874$ (6) Å. The crystal structure comprises an alternating stacking of puckered [LaTe] slabs and planar [Te] layers along [001]. The planar [Te] layer is dominated by dumbbell-shaped Te$_2^{2-}$ anions along an isolated Te$_2^{2-}$/Ca anion and a vacancy. The Te$_2^{2-}$ anions form an eight-membered ring enclosing the vacancy in the centre.

1. Chemical context

Chalcogenides $REX_{2-d}$ ($RE = Y, La$–Nd, Sm, Gd–Lu; $X = S$, Se, Te) of trivalent rare-earth metals comprise a large structural variety in a small compositional range $0 \leq d \leq 0.2$. This variety can mainly be attributed to the amount of vacancies as this strongly affects the final structural motif (Doert & Müller, 2016). All crystal structures share a common motif of alternating $[REX]$ and planar $[X]$ layers, related to their common aristotype, the structure of ZrSSi. Here, the same stacking arrangement is observed with a puckered [ZrS] slab and a planar [Si] layer, where an idealized square-planar [Si] layer is realized (Onken et al., 1964; Klein Haneveld & Jellinek, 1964). The chalcogenides, however, do not form a square-planar arrangement for electronic reasons, which can be understood by their charge-balanced formula: considering trivalent rare-earth metal cations only, the puckered [REX] slab bears a single positive charge per formula unit, which needs to be compensated by atoms of the planar [X] layer. This is achieved by forming dinuclear $X_2^{2-}$ anions in the stoichiometric dichalcogenides $REX_2$. The formation of such dumbbell-shaped anions results in a distortion from the ideal square-planar layer. Reducing the chalcogenide content results in the formation of vacancies inside the planar [X] layer, which in turn forces a reaction of the remaining atoms to balance the missing charge. Consequently, an isolated $X^{2-}$ anion per vacancy is formed to maintain a charge-balanced motif, adding two new constituting fragments to the planar layer. As vacancies are not randomly distributed within the layer, commensurate and incommensurately modulated superstructures are found (Doert & Müller, 2016). The structural chemistry of the corresponding sulfides and selenides has been thoroughly investigated, revealing several crystal structures that are observed for both chalcogens. The tellurides, however, do not always match the structures of their sulfur and selenium congeners, as shown for LaTe$_2$ (Stöwe, 2000a), CeTe$_2$ (Stöwe, 2000b) and PrTe$_2$ (Stöwe, 2000c). Discrepancies are also observed for the Te-deficient compound NdTe$_{1.89}$ (Stöwe,
However, the CeSe\textsubscript{1.9} type (Plambeck-Fischer et al., 1989) with a $\sqrt{5} \times \sqrt{5} \times 2$ supercell of the basic ZrSSi structure seems common to sulfides, selenides and tellurides. CeTe\textsubscript{1.9} was found to adopt this superstructure in space group $P4_2/n$ (No. 86) (Ijjaali & Ibers, 2006). The general motif of alternating stacks of [RET\textsubscript{e}] slabs and planar [Te] layers is preserved in this structure, the planar [Te] layer comprise four Te\textsuperscript{2–} anions surrounding a vacancy, resembling an eight-membered Te ring with alternating long and short distances. Four of these Te rings surround an isolated Te\textsuperscript{2–} anion in a pinwheel-like arrangement. Rationalizing this motif yields ten negative charges due to four Te\textsuperscript{2–} and a single Te\textsuperscript{3–} anion, balancing ten positive charges of each [RET\textsubscript{e}] layer. Here we report on the isotypic compound LaTe\textsubscript{1.9}, for which no structural characterization has been published yet.

2. Structural commentary

LaTe\textsubscript{1.9} crystallizes in space group $P4_2/n$ (No. 86) in the CeSe\textsubscript{1.9} structure type (Plambeck-Fischer et al., 1989) with $a = 10.1072$ (3) Å and $c = 18.2874$ (6) Å, corresponding to a $\sqrt{5} \times \sqrt{5} \times 2$ superstructure of the basic ZrSSi unit cell. As indicated above, two stacks of the basic arrangement are present in the structure of LaTe\textsubscript{1.9} as the Te-deficient planar [Te] layers are shifted by an $n$-glide against each other (Fig. 1). The La atoms are coordinated by eight Te atoms (La\textsubscript{2}), respectively nine Te atoms (La\textsubscript{1}, La\textsubscript{3}) forming a bicapped, respectively a tricapped trigonal prism. The La—Te distances within the slabs range from 3.2637 (2) to 3.3594 (2) Å and from 3.2944 (3) to 3.4480 (3) between the planar [Te] layer and La. Calculating the bond-valence sum $bvs$ (Brese & O’Keeffe, 1991) for each La site results in 2.99 valence units (v.u.) for La\textsubscript{1}, 3.06 v.u. for La\textsubscript{2} and 2.94 v.u. for La\textsubscript{3}, which are all very close to the expected value of +3 considering the previously discussed charge-balancing situation. The tellurium layer exhibits a pinwheel-like arrangement of four eight-membered Te squares surrounding a single Te\textsuperscript{2–} anion in its centre (Fig. 2), common to all compounds of the CeSe\textsubscript{1.9} type.

In view of the alternating short and long distances, the Te ring can be understood as being built up from four dinuclear Te\textsubscript{2} \textsuperscript{2–} anions enclosing a vacancy with alternating bonding and non-bonding distances of 2.9224 (3) and 3.1413 (3) Å, respectively.

In accordance with the charge balancing mentioned above and $Z = 20$, a structured formula of LaTe\textsubscript{1.9} can be written as [(La\textsuperscript{3+})\textsubscript{20}(Te\textsuperscript{2–})\textsubscript{20}] [(Te\textsuperscript{2–})\textsubscript{8}(Te\textsuperscript{2–})\textsubscript{2}]. This easily explains the anionic motifs and their quantity in the planar [Te] layer: Te5 and Te6 (both on Wyckoff site 8g) form the dumbbell-shaped Te\textsuperscript{2–} anions whereas Te4 (Wyckoff site 2b) represents the isolated Te\textsuperscript{2–} (Fig. 2).

3. Database survey

The CeSe\textsubscript{1.9} structure type (Plambeck-Fischer et al., 1989) is realized by several rare-earth metal sulfides and selenides but only by a few tellurides, CeTe\textsubscript{1.9} being one prominent example (Ijjaali & Ibers, 2006). The interatomic distances of LaTe\textsubscript{1.9} match those observed for CeTe\textsubscript{1.9} quite well, including the bonding and non-bonding distances in the planar [Te] layers [2.9224 (3) Å and 3.1413 (3) Å in LaTe\textsubscript{1.9} vs 2.9194 (5) Å and 3.1204 (5) Å in CeTe\textsubscript{1.9}]. However, the bonding Te—Te distances in these two compounds are considerably longer compared to compounds featuring (largely) isolated Te\textsuperscript{2–}. 

---

Figure 1
Crystal structure of LaTe\textsubscript{1.9} with displacement ellipsoids drawn at the 99.95% probability level. The stacking arrangement of puckered [LaTe] slabs and planar [Te] layers along [001] is shown.

Figure 2
[Te] layer of LaTe\textsubscript{1.9} with four Te\textsuperscript{2–} anions enclosing a vacancy each and surrounding an isolated Te\textsuperscript{2–} anion; displacement ellipsoids are drawn at the 99.95% probability level.
anions as constituting fragments, e.g. in \(\alpha\)-K\(_2\)Te\(_2\) (2.86 Å), \(\beta\)-K\(_2\)Te\(_2\) (2.790 (1) Å), Rb\(_2\)Te\(_2\) (2.78 Å) or GdTe\(_{1.8}\) (2.868 (1) Å) (Böttcher et al., 1993; Poddig et al., 2018).

4. Synthesis and crystallization

Crystals of LaTe\(_{1.9}\) were found as a byproduct during the investigation of the system La–Te in chemical transport experiments using iodine as transport agent. All preparation steps were carried out in an argon-filled (5.0, Praxair Deutschland GmbH, Düsseldorf, Germany) glove box (MBraun, Garching, Germany). Starting from the elements, 300 mg of a stoichiometric mixture of La (99.5%, MaTecK) and Te (Merck, >99.9%), reduced in H\(_2\) stream at 670 K) were ground and loaded into a silica ampule. A small amount of I\(_2\) was added inside the glove box before flame-sealing the ampule. After seven days, the ampule was cooled down to room temperature. A synthesis resulting in a phase pure product of LaTe\(_{1.9}\) has not yet been successful. The reason is most probably that two other Te-deficient compounds also exist in the composition range LaTe\(_{2.4}\) (0 ≤ \(\delta\) ≤ 0.2) along the stoichiometric ditelluride, namely LaTe\(_{1.94}\) (1) and LaTe\(_{1.82}\) (1) (Poddig & Doert, 2020; Poddig et al., 2020). To address the stability ranges of the individual phases, the chalcogen vapor pressures and temperatures have to be evaluated and controlled precisely during synthesis (Müller et al., 2010).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All investigated crystals of LaTe\(_{1.9}\) were found as reticular merohedric twins with a twin index \(n = 5\). On a first glance, the diffraction patterns seem to suggest a large tetragonal unit cell with apparent lattice parameters of \(a = 22.6211\) (6) Å and \(c = 18.3135\) (5) Å, corresponding to a 50-fold superstructure of the basic ZrSSi structure (Fig. 3). Similar apparent supercells have been reported for the sulfides SmS\(_{1.9}\) (Tamazyan et al., 2000) or TmS\(_{1.9}\) (Müller et al., 2012), and can be explained by twinning along the mirror planes in (100) and (110) of the twin lattice. A schematic scheme drawn along [001] is depicted in Fig. 3, illustrating the lattices of each domain. The corresponding twin law calculated by the diffractometer software (Bruker, 2016) corresponds to the twin law derived for SmS\(_{1.9}\) (0.6 –0.8 0 –0.8 –0.6 0 0 0 1). Both domains were handled during the process of integrating and correcting the data, and the refinements were performed on a HKLF5 format file. The twin ratio of the two domains calculated by SHELXL is 0.57 (1):43 (1).

Funding information

Funding for this research was provided by: Deutsche Forschungsgemeinschaft (grant No. Do 560/1).

![Figure 3](image-url)
References

Böttcher, P., Getzschmann, J. & Keller, R. (1993). Z. Anorg. Allg. Chem. 619, 476–488.

Brandenburg, K. (2018). DIAMOND. Crystal Impact GbR, Bonn, Germany.

Brese, N. E. & O’Keeffe, M. (1991). Acta Cryst. B47, 192–197.

Bruker (2012). TWINABS. Bruker AXS, Madison, WI, USA.

Bruker (2016). APEX2 and SAINT. Bruker AXS, Madison, Wisconsin, USA.

Doert, T. & Müller, C. J. (2016). Reference Module in Chemistry, Molecular Sciences and Chemical Engineering. Amsterdam: Elsevier.

Ijjaali, I. & Ibers, J. A. (2006). J. Solid State Chem. 179, 3456–3460.

Klein Haneveld, A. & Jellinek, F. (1964). Recl Trav. Chim. Pays Bas, 83, 776–783.

Müller, C. J., Schwarz, U. & Doert, T. (2012). Z. Anorg. Allg. Chem. 638, 2477–2484.

Müller, C. J., Schwarz, U., Schmidt, P., Schnelle, W. & Doert, T. (2010). Z. Anorg. Allg. Chem. 636, 947–953.

Onken, H., Vierheilig, K. & Hahn, H. (1964). Z. Anorg. Allg. Chem. 333, 267–279.

Plambeck-Fischer, P., Abriel, W. & Urland, W. (1989). J. Solid State Chem. 78, 164–169.

Poddig, H. & Doert, T. (2020). Acta Cryst. B76, 1092–1099.

Poddig, H., Donath, T., Gebauer, P., Finzel, K., Kohout, M., Wu, Y., Schmidt, P. & Doert, T. (2018). Z. Anorg. Allg. Chem. 644, 1886–1896.

Poddig, H., Finzel, K. & Doert, T. (2020). Acta Cryst. C76, 530–540.

Sheldrick, G. M. (2015a). Acta Cryst. A71, 3–8.

Sheldrick, G. M. (2015b). Acta Cryst. C71, 3–8.

Stöwe, K. (2000a). J. Solid State Chem. 149, 155–166.

Stöwe, K. (2000b). J. Alloys Compd. 307, 101–110.

Stöwe, K. (2000c). Z. Anorg. Allg. Chem. 626, 803–811.

Stöwe, K. (2001). Z. Kristallogr. Cryst. Mater. 216, 215–224.

Tamazyan, R., Arnold, H., Molchanov, V., Kuzmicheva, G. & Vasileva, I. (2000). Z. Kristallogr. Cryst. Mater. 215, 346–351.

Westrip, S. P. (2010). J. Appl. Cryst. 43, 920–925.

562 Poddig and Doert • LaTe$_{1.90}$
supporting information

Acta Cryst. (2022). E78, 559-562  [https://doi.org/10.1107/S2056989022004844]

LaTe$_{1.9}$: a tenfold superstructure of the ZrSSi type

Hagen Poddig and Thomas Doert

Computing details

Data collection: APEX2 (Bruker, 2016); cell refinement: SAINT (Bruker, 2016); data reduction: SAINT (Bruker, 2016); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: SHELXL (Sheldrick, 2015b); molecular graphics: DIAMOND (Brandenburg, 2018); software used to prepare material for publication: publCIF (Westrip, 2010).

Lanthanum telluride (1/1.9)

Crystal data

LaTe$_{1.90}$  
$M_r = 381.35$  
Tetragonal, $P4_2/n$  
$a = 10.1072 (3)$ Å  
c = 18.2874 (6) Å  
$V = 1868.16 (13)$ Å$^3$  
Z = 20  
$F(000) = 3116$

$D_x = 6.779$ Mg m$^{-3}$  
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å  
Cell parameters from 9906 reflections  
$\theta = 3.6$–46.4°  
$\mu = 25.70$ mm$^{-1}$  
$T = 100$ K  
Block, black  
0.11 × 0.08 × 0.04 mm

Data collection

Bruker APEXII CCD  
diffractionometer  
Radiation source: sealed X-ray tube  
Graphite monochromator  
$\varphi$ and $\omega$ scans  
Absorption correction: multi-scan  
(TWINABS; Bruker, 2012)  
$T_{\text{min}} = 0.399$, $T_{\text{max}} = 0.749$

7850 measured reflections  
7850 independent reflections  
5970 reflections with $I > 2\sigma(I)$  
$R_{int} = 0.055$

$\theta_{\text{max}} = 45.3^\circ$, $\theta_{\text{min}} = 2.9^\circ$

Refinement

Refinement on $F^2$  
Least-squares matrix: full  
$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.061$

$S = 1.12$

7850 reflections  
69 parameters  
0 restraints

Primary atom site location: iterative  
Secondary atom site location: difference Fourier map  
Extinction correction: SHELXL-2016/6  
(Sheldrick 2015b), $F^2 = kF[c(1+0.001xFc^2/\sin(2\theta)]^{1/4}$  
Extinction coefficient: 0.001129 (18)
**Special details**

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refined as a 2-component twin.

**Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)**

|       | x    | y    | z    | \(U_{iso}^*\)/\(U_{eq}\) |
|-------|------|------|------|--------------------------|
| La1   | 0.250000 | −0.250000 | 0.38287 (2) | 0.00695 (4) |
| La2   | 0.14760 (2) | 0.05231 (2) | 0.10752 (2) | 0.00710 (3) |
| La3   | −0.15137 (2) | −0.04353 (2) | 0.38089 (2) | 0.00696 (3) |
| Te1   | −0.250000 | 0.250000 | 0.43532 (2) | 0.00722 (4) |
| Te2   | 0.14951 (2) | 0.05177 (2) | 0.43621 (2) | 0.00726 (3) |
| Te3   | −0.15255 (2) | −0.04952 (2) | 0.07093 (2) | 0.00722 (3) |
| Te4   | −0.250000 | −0.250000 | 0.250000 | 0.00773 (5) |
| Te5   | −0.02702 (2) | 0.16873 (2) | 0.25027 (2) | 0.00992 (3) |
| Te6   | 0.06086 (2) | −0.12938 (2) | 0.24930 (2) | 0.00770 (3) |

**Atomic displacement parameters (Å²)**

|       | \(U_{11}\) | \(U_{22}\) | \(U_{33}\) | \(U_{12}\) | \(U_{13}\) | \(U_{23}\) |
|-------|------------|------------|------------|------------|------------|------------|
| La1   | 0.00683 (8) | 0.00672 (8) | 0.00729 (7) | 0.00054 (6) | 0.0000 | 0.000 |
| La2   | 0.00723 (6) | 0.00691 (6) | 0.00715 (5) | 0.00000 (5) | 0.00005 (4) | 0.00083 (4) |
| La3   | 0.00657 (6) | 0.00689 (6) | 0.00744 (5) | 0.00015 (5) | −0.00001 (4) | −0.00070 (4) |
| Te1   | 0.00701 (9) | 0.00696 (9) | 0.00769 (8) | 0.00009 (7) | 0.000 | 0.000 |
| Te2   | 0.00684 (7) | 0.00726 (7) | 0.00767 (5) | −0.00005 (6) | 0.00002 (5) | −0.00037 (4) |
| Te3   | 0.00712 (7) | 0.00697 (7) | 0.00756 (5) | 0.00007 (6) | 0.00001 (5) | 0.00005 (5) |
| Te4   | 0.00815 (7) | 0.00815 (7) | 0.00690 (11) | 0.000 | 0.000 |
| Te5   | 0.01106 (7) | 0.01167 (7) | 0.00702 (6) | 0.00045 (6) | 0.00031 (6) | −0.00005 (5) |
| Te6   | 0.00881 (7) | 0.00761 (6) | 0.00667 (5) | 0.00034 (5) | −0.00003 (5) | −0.00016 (5) |

**Geometric parameters (Å, º)**

|       | La1—Te3 | La2—Te6 | La2—Te1 | La3—Te4 | La3—Te6 | La3—Te2 |
|-------|---------|---------|---------|---------|---------|---------|
| La1—Te3 | 3.2938 (2) | 3.2960 (2) | 3.3198 (2) | 3.3284 (2) | 3.3361 (3) | 3.3384 (2) |
| La1—Te1 | 3.2938 (2) | 3.3284 (3) | 3.3637 (3) | 3.3284 (2) | 3.3361 (3) | 3.3384 (2) |
| La1—Te6 | 3.3293 (3) | 3.3329 (2) | 3.3284 (2) | 3.3361 (3) | 3.3384 (2) | 3.3465 (3) |
| La1—Te2 | 3.3594 (2) | 3.3594 (2) | 3.3384 (2) | 3.3384 (2) | 3.3384 (2) | 3.3384 (2) |
| La1—Te5 | 3.4179 (3) | 3.4179 (3) | 3.4179 (3) | 3.4179 (3) | 3.4179 (3) | 3.4179 (3) |
| La2—Te3 | 3.2637 (2) | 3.2637 (2) | 3.2637 (2) | 3.2637 (2) | 3.2637 (2) | 3.2637 (2) |
| La2—Te2 | 3.2649 (3) | 3.2649 (3) | 3.2649 (3) | 3.2649 (3) | 3.2649 (3) | 3.2649 (3) |
| La2—Te1 | 3.2726 (3) | 3.2726 (3) | 3.2726 (3) | 3.2726 (3) | 3.2726 (3) | 3.2726 (3) |
| La2—Te5 | 3.2920 (3) | 3.2920 (3) | 3.2920 (3) | 3.2920 (3) | 3.2920 (3) | 3.2920 (3) |
La$_2$—Te$_5^i$ 3.2944 (3) Te$_5$—Te$_6$ 3.1413 (3)

| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|-----------------------|--------------|-----------------------|--------------|
| Te$_3^i$—La$_1$—Te$_3^ii$ | 150.272 (10) | Te$_2^iii$—La$_3$—Te$_3^ii$ | 73.330 (5) |
| Te$_3^i$—La$_1$—Te$_1^iii$ | 75.136 (5)   | Te$_2$—La$_3$—Te$_3^ii$ | 84.571 (6)  |
| Te$_3^i$—La$_1$—Te$_1^ii$ | 75.136 (5)   | Te$_1$—La$_3$—Te$_6^ii$ | 74.669 (6)  |
| Te$_3^i$—La$_1$—Te$_6$   | 127.287 (6)  | Te$_4$—La$_3$—Te$_6^ii$ | 59.908 (4)  |
| Te$_3^ii$—La$_1$—Te$_6$  | 76.715 (5)   | Te$_3^ii$—La$_3$—Te$_6^ii$ | 72.455 (5)  |
| Te$_1^iii$—La$_1$—Te$_6$ | 137.132 (4)  | Te$_6$—La$_3$—Te$_6^ii$ | 89.696 (6)  |
| Te$_3$—La$_1$—Te$_6^w$  | 76.715 (5)   | Te$_2^ii$—La$_3$—Te$_6^ii$ | 135.020 (7) |
| Te$_3^i$—La$_1$—Te$_6^w$ | 127.288 (6)  | Te$_2$—La$_3$—Te$_6^ii$ | 135.283 (7) |
| Te$_1^ii$—La$_1$—Te$_6^w$ | 137.132 (4)  | Te$_3^ii$—La$_3$—Te$_6^ii$ | 131.586 (6) |
| Te$_6$—La$_1$—Te$_6^w$  | 85.735 (8)   | Te$_1$—La$_3$—Te$_5$ | 76.027 (6)  |
| Te$_3^i$—La$_1$—Te$_2$  | 85.364 (5)   | Te$_4$—La$_3$—Te$_5$ | 90.060 (6)  |
| Te$_3^ii$—La$_1$—Te$_2$ | 86.094 (5)   | Te$_3^iii$—La$_3$—Te$_5$ | 135.955 (7) |
| Te$_1^iii$—La$_1$—Te$_2^iv$ | 73.124 (5)  | Te$_6$—La$_3$—Te$_5$ | 55.118 (5)  |
| Te$_6$—La$_1$—Te$_2^iv$  | 135.915 (6)  | Te$_2^ii$—La$_3$—Te$_5$ | 134.911 (7) |
| Te$_6^w$—La$_1$—Te$_2^iv$ | 72.977 (5)   | Te$_2$—La$_3$—Te$_5$ | 72.489 (5)  |
| Te$_3^i$—La$_1$—Te$_2$  | 86.094 (5)   | Te$_3^ii$—La$_3$—Te$_5$ | 129.745 (6) |
| Te$_3^ii$—La$_1$—Te$_2$ | 85.363 (5)   | Te$_6^w$—La$_3$—Te$_5$ | 64.015 (6)  |
| Te$_1^iii$—La$_1$—Te$_2$ | 73.123 (5)   | La$_3$—Te$_1$—La$_3^viii$ | 144.714 (11) |
| Te$_6$—La$_1$—Te$_2$  | 72.977 (5)   | La$_3$—Te$_1$—La$_2^ii$ | 85.769 (5)  |
| Te$_6^w$—La$_1$—Te$_2$ | 135.915 (6)  | La$_3^vii$—Te$_1$—La$_2^ii$ | 86.028 (4) |
| Te$_2^iv$—La$_1$—Te$_2$ | 146.246 (10) | La$_3$—Te$_1$—La$_2^v$ | 86.029 (4)  |
| Te$_3^i$—La$_1$—Te$_5^i$ | 126.928 (6)  | La$_3^vii$—Te$_1$—La$_2^v$ | 85.769 (4)  |
| Te$_3^ii$—La$_1$—Te$_5^i$ | 76.389 (5)   | La$_2^ii$—Te$_1$—La$_2^ii$ | 152.703 (10) |
| Te$_1^iii$—La$_1$—Te$_5^ii$ | 135.428 (4)  | La$_3$—Te$_1$—La$_1^iii$ | 107.643 (5) |
| Te$_6$—La$_1$—Te$_5^ii$ | 65.244 (6)   | La$_3^vii$—Te$_1$—La$_1^ii$ | 107.643 (5) |
| Te$_6^w$—La$_1$—Te$_5^ii$ | 51.284 (5)   | La$_2^ii$—Te$_1$—La$_1^ii$ | 103.648 (5) |
| Te$_2^v$—La$_1$—Te$_5^vii$ | 71.386 (5)  | La$_2^v$—Te$_1$—La$_1^iii$ | 103.648 (5) |
| Te$_2$—La$_1$—Te$_5^i$  | 137.123 (7)  | La$_2^v$—Te$_2$—La$_2^v$ | 86.685 (6)  |
| Te$_3^i$—La$_1$—Te$_5^i$ | 76.389 (5)   | La$_2$—Te$_2$—La$_3^iii$ | 104.300 (6) |
| Te$_3^ii$—La$_1$—Te$_5^i$ | 126.928 (6)  | La$_2^v$—Te$_2$—La$_3^iii$ | 105.511 (6) |
| Te$_1^iii$—La$_1$—Te$_5^i$ | 135.428 (4)  | La$_2$—Te$_2$—La$_3^ii$ | 148.230 (7) |
| Te$_6$—La$_1$—Te$_5^i$  | 51.283 (5)   | La$_2$—Te$_2$—La$_3$ | 85.472 (6)  |
| Te$_6^w$—La$_1$—Te$_5^i$ | 65.243 (6)   | La$_3^vii$—Te$_2$—La$_3$ | 107.465 (6) |
| Te$_2^v$—La$_1$—Te$_5^vii$ | 137.122 (7)  | La$_2^v$—Te$_2$—La$_1$ | 85.364 (5)  |
| Te$_2$—La$_1$—Te$_5^i$  | 71.387 (5)   | La$_2^v$—Te$_2$—La$_1$ | 149.063 (7) |
| Te$_5^ii$—La$_1$—Te$_5^i$ | 89.144 (9)   | La$_3^vii$—Te$_2$—La$_1$ | 105.424 (7) |
| Te$_3^i$—La$_2$—Te$_2^i$ | 76.566 (5)   | La$_3$—Te$_2$—La$_1$ | 85.737 (5)  |
| Te$_3^i$—La$_2$—Te$_3$  | 78.875 (7)   | La$_2^v$—Te$_3$—La$_2$ | 101.125 (7) |
| Te$_2^v$—La$_2$—Te$_3$  | 88.008 (6)   | La$_2^v$—Te$_3$—La$_1^vi$ | 105.604 (7) |
| Te$_3^i$—La$_2$—Te$_2^i$ | 75.263 (5)   | La$_2$—Te$_3$—La$_1^vi$ | 86.313 (5)  |
| Te$_2^v$—La$_2$—Te$_2^i$ | 86.496 (6)   | La$_2$—Te$_3$—La$_3^ii$ | 104.549 (6) |
| Te$_3$—La$_2$—Te$_2^i$  | 154.134 (7)  | La$_2$—Te$_3$—La$_3^ii$ | 85.690 (6)  |
| Te$_3^i$—La$_2$—Te$_5^i$ | 141.133 (7)  | La$_1^v$—Te$_3$—La$_3^ii$ | 149.757 (7) |
| Te$_2^v$—La$_2$—Te$_5^i$ | 125.814 (7)  | La$_2$—Te$_3$—La$_3^ii$ | 105.889 (6) |
| Te$_3$—La$_2$—Te$_5^i$  | 127.388 (7)  | La$_2$—Te$_3$—La$_3^vii$ | 152.986 (8) |
| Te$_2^v$—La$_2$—Te$_5^i$ | 75.182 (6)   | La$_1^v$—Te$_3$—La$_3^vii$ | 86.610 (5)  |
Table of bond angles (°) and distances (Å) for Te3v—La2—Te6, La3vi—Te3—La3vii, and other bond pairs:

| Bond Pair                      | Angle    | Distance |
|--------------------------------|----------|----------|
| Te3v—La2—Te6                  | 141.795  | (7)      |
| Te2vi—La2—Te6                 | 128.902  | (6)      |
| Te3—La2—Te6                   | 74.873   | (6)      |
| Te2—La2—Te6                   | 127.073  | (7)      |
| Te5—La2—Te6                   | 52.645   | (6)      |
| Te3—La2—Te1ii                 | 75.603   | (6)      |
| Te2vi—La2—Te1ii               | 152.164  | (7)      |
| Te3—La2—Te1i                  | 87.208   | (5)      |
| Te2—La2—Te1i                  | 85.964   | (5)      |
| Te5—La2—Te1i                  | 77.677   | (6)      |
| Te6—La2—Te1i                  | 75.863   | (6)      |
| Te3—La2—Te5                   | 141.908  | (8)      |
| Te2vi—La2—Te5                 | 73.230   | (6)      |
| Te3—La2—Te5                   | 77.427   | (6)      |
| Te2—La2—Te5                   | 124.638  | (7)      |
| Te5—La2—Te5                   | 76.593   | (7)      |
| Te6—La2—Te5                   | 56.276   | (6)      |
| Te1—La2—Te5                   | 131.965  | (7)      |
| Te1—La3—Te4                   | 133.902  | (7)      |
| Te1—La3—Te3viii               | 86.745   | (5)      |
| Te4—La3—Te3viii               | 73.231   | (5)      |
| Te1—La3—Te6                   | 130.412  | (7)      |
| Te4—La3—Te6                   | 60.731   | (4)      |
| Te3viii—La3—Te6               | 133.378  | (6)      |
| Te1—La3—Te2iii                | 73.811   | (6)      |
| Te4—La3—Te2iii                | 134.830  | (7)      |
| Te3viii—La3—Te2iii            | 74.503   | (5)      |
| Te6—La3—Te2iii                | 135.279  | (7)      |
| Te1—La3—Te2                   | 85.654   | (5)      |
| Te4—La3—Te2                   | 132.068  | (6)      |
| Te3viii—La3—Te2               | 147.001  | (7)      |
| Te6—La3—Te2                   | 73.072   | (6)      |
| Te2iii—La3—Te2                | 72.535   | (6)      |
| Te1—La3—Te3viii               | 147.141  | (7)      |
| Te4—La3—Te3viii               | 72.959   | (5)      |
| Te3viii—La3—Te3vii            | 84.626   | (6)      |
| Te6—La3—Te3viii               | 75.783   | (6)      |

Symmetry codes: (i) y+1/2, x, z+1/2; (ii) y, −x−1/2, −z+1/2; (iii) −x, −y, z+1; (iv) −x+1/2, −y−1/2, z; (v) −x, −y, z; (vi) y, −x+1/2, −z+1/2; (vii) −y+1/2, x, z+1/2; (viii) −x−1/2, −y+1/2, z; (ix) −x+1/2, −y−1/2, z.