

The low-symmetry lanthanum(III) oxotellurate(IV), La₁₀Te₁₂O₃₉

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Te}-\text{O}) = 0.007$ Å; disorder in main residue; R factor = 0.042; wR factor = 0.064; data-to-parameter ratio = 30.9.

Single crystals of decalanthanum(III) dodecaoxotellurate(IV), La₁₀Te₁₂O₃₉, were obtained by reacting La₂O₃ and TeO₂ in a CsCl flux. Its crystal structure can be viewed as a three-dimensional network of corner- and edge-sharing LaO₈ polyhedra with Te^{IV} atoms filling the interstitial sites. The Te^{IV} atoms with their 5s² electron lone pairs distort the LaO₈ polyhedra through variable Te—O bonds. Among the six unique Te sites, four of them define empty channels extending parallel to the a axis. The formation of these channels is a result of the stereochemically active electron lone pairs on the Te^{IV} atoms. The atomic arrangement of the Te—O units can be understood on the basis of the valence shell electron pair repulsion (VSEPR) model. A certain degree of disorder is observed in the crystal structure. As a result, one of the five different La sites is split into two positions with an occupancy ratio of 0.875 (2):0.125 (2). Also, one of the oxygen sites is split into two positions in a 0.559 (13):0.441 (13) ratio, and one O site is half-occupied. Such disorder was observed in all measured La₁₀Te₁₂O₃₉ crystals.

Related literature

For the structures of related rare-earth oxotellurates(IV), see: Castro *et al.* (1990); Weber *et al.* (2001); Meier *et al.* (2009). For synthetic details, see: Weber & Schleid (2000). For standardization of structural data, see: Gelato & Parthé (1987). For the VSEPR model, see: Gillespie (1970). For the bond-valence method, see: Brown (2009).

Experimental

Crystal data

La ₁₀ Te ₁₂ O ₃₉	$\gamma = 93.13$ (3)°
$M_r = 3544.30$	$V = 1007.3$ (3) Å ³
Triclinic, $P\bar{1}$	$Z = 1$
$a = 5.6856$ (11) Å	Mo $K\alpha$ radiation
$b = 12.621$ (3) Å	$\mu = 18.98$ mm ⁻¹
$c = 14.402$ (3) Å	$T = 293$ K
$\alpha = 95.53$ (3)°	$0.12 \times 0.04 \times 0.02$ mm
$\beta = 100.88$ (3)°	

Data collection

Stoe IPDSII diffractometer	18743 measured reflections
Absorption correction: numerical (<i>X-SHAPE</i> and <i>X-RED32</i> ; Stoe, 2004)	8922 independent reflections
$T_{\min} = 0.256$, $T_{\max} = 0.702$	5110 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.063$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	289 parameters
$wR(F^2) = 0.064$	$\Delta\rho_{\max} = 3.71$ e Å ⁻³
$S = 0.77$	$\Delta\rho_{\min} = -3.98$ e Å ⁻³
8922 reflections	

Data collection: *X-AREA* (Stoe, 2004); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Crystal Impact, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2737).

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supporting information

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The low-symmetry lanthanum(III) oxotellurate(IV), $\text{La}_{10}\text{Te}_{12}\text{O}_{39}$

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S1. Comment

A number of rare-earth(III) oxotellurates(IV), including $\text{Dy}_2\text{Te}_3\text{O}_9$ (Meier *et al.*, 2009), $\text{Nd}_2\text{Te}_4\text{O}_{11}$ (Castro *et al.*, 1990) and $\text{Ho}_2\text{Te}_5\text{O}_{13}$ (Weber *et al.*, 2001), have been prepared and structurally characterized. Despite their different compositions, these compounds all contain tellurium atoms in the oxidation state +IV. The remaining two electrons on the Te^{IV} atoms usually form stereo-chemically active but chemically non-bonding electron lone pairs. The local atomic arrangements around these Te^{IV} atoms with electron lone pairs can be understood on basis of the 'Valence Shell Electron Pair Repulsion' (VSEPR) model (Gillespie, 1970). As the local symmetry of the Te^{IV} sites is reduced by the lone pairs, these compounds usually adopt low-symmetry space groups, *e.g.* $C2/c$ for $\text{Nd}_2\text{Te}_4\text{O}_{11}$, $P\bar{1}$ for $\text{Ho}_2\text{Te}_5\text{O}_{13}$ or $P2_1/c$ for $\text{Dy}_2\text{Te}_3\text{O}_9$. The title compound, $\text{La}_{10}\text{Te}_{12}\text{O}_{39}$, can be considered as another member of the rare-earth(III) oxotellurates(IV) family. Structural similarities can be observed between $\text{La}_{10}\text{Te}_{12}\text{O}_{39}$ and other rare-earth(III) oxotellurates(IV), including the distorted LaO_8 polyhedra and a number of different Te–O structural motifs. Among the six Te atoms in the unit cell, four of them define empty channels parallel to the *a*-axis, while the other two fill the interstitial positions between the LaO_8 polyhedra (Fig. 1).

If Te–O distances ≤ 2.03 Å (sum of the Te and O covalent radii) are considered as primary Te–O bonds, three TeO_3 units (for Te1, Te4 and Te6) can be identified. Also, a fourth long Te–O interaction is observed for each of these three Te atoms (the fourth oxygen atoms is 2.852 (6) Å from Te1, 2.923 (8) Å from Te4 and 2.802 (6) Å from Te6). Bond valence sum calculations (Brown, 2009) show a minimal contribution from these long interactions; when these interactions are discarded, the bond valence sums for the 3-coordinated Te1, Te4 and Te6 atoms are close to 4.0 valence units (v.u.). The other three Te atoms (Te2, Te3 and Te5) display shorter secondary Te–O interactions (≤ 2.5 Å), which allow them to form TeO_4 units in distorted seesaw configurations. The bond valence sums indicate significant contributions from these interactions. For these TeO_4 units, bond valence sum are 3.9 v.u., 3.9 v.u and 4.4 v.u for Te2, Te3 and Te5, respectively. Such results are consistent with the assignment of oxidation state +IV for the Te atoms.

The competition between the Te2 and Te5 atoms to form stronger interactions with the bridging oxygen atom (O19) also causes disorder on the oxygen site. As a result, O19 is split into two separated oxygen positions (O191 and O192) to account for the electron density distribution. In addition to the disordered oxygen sites, one of the lanthanum sites (La5) is also described by split positions (La51 and La52). Such disorder could be a consequence of the asymmetric environment in the distorted LaO_8 polyhedron.

S2. Experimental

Single crystals of $\text{La}_{10}\text{Te}_{12}\text{O}_{39}$ were obtained by reacting La_2O_3 (99.99 wt. %, Rhône-Poulenc, pre-fired at 1273 K for 12 h) and TeO_2 (99.99%, Johnson Matthey Electronics) in a CsCl (99.9%, Alfa-Aesar) flux (Weber & Schleid, 2000). In total, 0.1 gram of the La_2O_3 and TeO_2 powder with the 1:2 molar ratio were ground and mixed with 1.9 grams of CsCl. The sample mixture was placed in an alumina crucible, which was sealed in a silica tube under vacuum. The sample was

heated to 1273 K at a rate of 50 K/h. After holding at 1273 K for 72 h, the temperature was then slowly decreased to 1073 K at a rate of 5 K/hour. After annealing at 1073 K for 20 h, the sample was quenched in air. Transparent, colorless, needle-shaped single crystals were obtained by washing away the salt flux with distilled water and ethanol.

S3. Refinement

The structure was standardized by using the *STRUCTURE TIDY* program (Gelato & Parthé, 1987). Two pairs of split positions, La51/La52 and O191/O192 were modelled to account for the observed electron density distribution. Between each pair of split sites, the sum of their occupancies was constrained to 100%, while the isotropic or anisotropic displacement parameters were equalized using the EADP command. The occupancies of each site was extracted from the refinement. Deficiency on the O20 site was observed during the refinement. The occupancy of the O20 site was later assigned to 50% to account for charge balance. The remaining maximum and minimum electron densities ($3.71 \text{ e} \cdot \text{\AA}^{-3}$ and $-3.98 \text{ e} \cdot \text{\AA}^{-3}$) are 0.62 \AA and 0.24 \AA , respectively, from atom Te5.

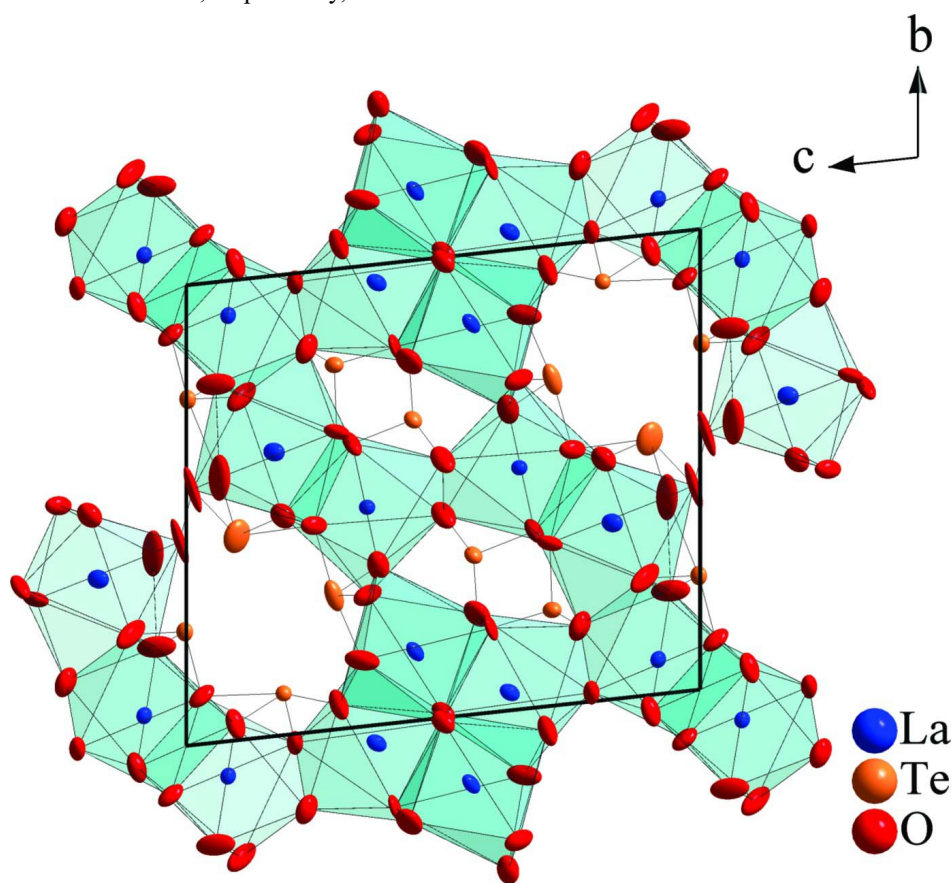


Figure 1

The crystal structure of $\text{La}_{10}\text{Te}_{12}\text{O}_{39}$ represented with displacement ellipsoids at the 90% probability level.

Decalanthanum dodecatellurium triacontnonaoxide

Crystal data

$\text{La}_{10}\text{Te}_{12}\text{O}_{39}$

$M_r = 3544.30$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 5.6856 (11) \text{ \AA}$

$b = 12.621 (3) \text{ \AA}$

$c = 14.402 (3) \text{ \AA}$

$\alpha = 95.53 (3)^\circ$

$\beta = 100.88 (3)^\circ$
 $\gamma = 93.13 (3)^\circ$
 $V = 1007.3 (3) \text{ \AA}^3$
 $Z = 1$
 $F(000) = 1506$
 $D_x = 5.843 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 18743 reflections
 $\theta = 2.9\text{--}36.9^\circ$
 $\mu = 18.98 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
 Needle, colourless
 $0.12 \times 0.04 \times 0.02 \text{ mm}$

Data collection

Stoe IPDSII
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω -scan
 Absorption correction: numerical
 (*X-SHAPE* and *X-RED32*; Stoe, 2004)
 $T_{\min} = 0.256$, $T_{\max} = 0.702$

18743 measured reflections
 8922 independent reflections
 5110 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.063$
 $\theta_{\max} = 36.3^\circ$, $\theta_{\min} = 2.9^\circ$
 $h = -9 \rightarrow 6$
 $k = -21 \rightarrow 20$
 $l = -23 \rightarrow 23$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.064$
 $S = 0.77$
 8922 reflections
 289 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 $w = 1/[\sigma^2(F_o^2) + (0.0122P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 3.71 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -3.98 \text{ e \AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00195 (3)

Special details

Experimental. A numerical absorption correction was based on the crystal shape that was originally derived from the optical face indexing but later optimized against equivalent reflections using Stoe *X-SHAPE* software (Stoe & Cie GmbH, 2004)

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.42088 (10)	0.52484 (4)	0.35191 (3)	0.00809 (10)	
La2	0.54271 (10)	0.15044 (4)	0.55453 (3)	0.01179 (12)	
La3	0.79356 (10)	0.07556 (4)	0.08168 (3)	0.00813 (9)	
La4	0.81948 (10)	0.38287 (4)	0.17100 (4)	0.01151 (11)	
La51	0.93544 (12)	0.03921 (6)	0.37049 (5)	0.01013 (15)	0.875 (2)
La52	0.9564 (9)	0.0092 (4)	0.3946 (4)	0.01013 (15)	0.125 (2)
Te1	0.03902 (11)	0.34576 (4)	0.44123 (4)	0.01010 (11)	

Te2	0.10966 (12)	0.29104 (6)	0.71241 (4)	0.01761 (14)	
Te3	0.22321 (11)	0.24798 (5)	0.00280 (4)	0.00909 (11)	
Te4	0.48089 (10)	0.20819 (4)	0.28804 (4)	0.01029 (11)	
Te5	0.33718 (14)	0.55670 (7)	0.09840 (5)	0.02424 (16)	
Te6	0.28887 (10)	0.90925 (4)	0.18953 (3)	0.00793 (10)	
O1	0.0464 (12)	0.8560 (5)	0.3423 (5)	0.0228 (15)	
O2	0.0751 (13)	0.2551 (6)	0.1077 (5)	0.0248 (15)	
O3	0.0812 (11)	0.3836 (5)	0.3226 (4)	0.0165 (13)	
O4	0.0853 (11)	0.1040 (5)	0.9697 (4)	0.0157 (13)	
O5	0.0957 (12)	0.0194 (5)	0.2117 (4)	0.0157 (13)	
O6	0.1285 (13)	0.6544 (6)	0.3738 (4)	0.0217 (14)	
O7	0.1599 (13)	0.5237 (5)	0.1880 (4)	0.0202 (14)	
O8	0.1863 (14)	0.2177 (6)	0.4339 (5)	0.0243 (15)	
O9	0.2484 (11)	0.0094 (5)	0.4996 (4)	0.0153 (13)	
O10	0.3008 (13)	0.4396 (6)	0.4992 (4)	0.0238 (16)	
O11	0.3612 (12)	0.2841 (5)	0.6470 (4)	0.0193 (13)	
O12	0.4366 (11)	0.9645 (5)	0.0960 (4)	0.0166 (12)	
O13	0.4386 (16)	0.4258 (8)	0.0647 (5)	0.039 (2)	
O14	0.4707 (11)	0.0531 (5)	0.7030 (4)	0.0195 (14)	
O15	0.5313 (11)	0.2219 (5)	0.0575 (5)	0.0253 (16)	
O16	0.5651 (11)	0.3536 (5)	0.2926 (4)	0.0139 (12)	
O17	0.6547 (11)	0.1833 (5)	0.4068 (4)	0.0139 (12)	
O18	0.7421 (12)	0.1666 (6)	0.2342 (4)	0.0207 (13)	
O191	0.290 (2)	0.4482 (9)	0.7515 (8)	0.0153 (18)	0.559 (13)
O192	0.382 (3)	0.4438 (11)	0.8010 (10)	0.0153 (18)	0.441 (13)
O20	0.916 (3)	0.4450 (15)	0.0126 (8)	0.032 (4)	0.50

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0086 (2)	0.0071 (2)	0.00811 (18)	0.00113 (17)	0.00047 (17)	0.00086 (15)
La2	0.0160 (3)	0.0123 (2)	0.0099 (2)	0.0065 (2)	0.0060 (2)	0.00511 (16)
La3	0.0085 (2)	0.00864 (19)	0.00750 (17)	0.00180 (17)	0.00207 (15)	0.00023 (14)
La4	0.0087 (2)	0.0109 (2)	0.0138 (2)	0.00191 (17)	-0.00131 (18)	0.00210 (17)
La51	0.0097 (2)	0.0098 (3)	0.0121 (3)	0.0027 (2)	0.0034 (2)	0.0037 (2)
La52	0.0097 (2)	0.0098 (3)	0.0121 (3)	0.0027 (2)	0.0034 (2)	0.0037 (2)
Te1	0.0108 (2)	0.0096 (2)	0.0100 (2)	-0.0011 (2)	0.00199 (18)	0.00261 (17)
Te2	0.0136 (3)	0.0306 (4)	0.0117 (2)	0.0098 (3)	0.0051 (2)	0.0082 (2)
Te3	0.0073 (2)	0.0111 (2)	0.00840 (19)	0.0012 (2)	0.00017 (18)	0.00111 (17)
Te4	0.0113 (2)	0.0080 (2)	0.0109 (2)	-0.00019 (19)	0.00045 (18)	0.00099 (16)
Te5	0.0210 (4)	0.0329 (4)	0.0213 (3)	0.0096 (3)	0.0112 (3)	-0.0031 (3)
Te6	0.0080 (2)	0.0077 (2)	0.00793 (19)	0.00001 (18)	0.00129 (18)	0.00082 (16)
O1	0.015 (3)	0.014 (3)	0.037 (4)	0.002 (2)	-0.004 (3)	0.008 (3)
O2	0.028 (4)	0.023 (4)	0.025 (3)	-0.007 (3)	0.019 (3)	-0.011 (3)
O3	0.016 (3)	0.019 (3)	0.012 (2)	-0.008 (2)	-0.003 (2)	0.008 (2)
O4	0.012 (3)	0.014 (3)	0.019 (3)	-0.003 (2)	0.002 (2)	-0.007 (2)
O5	0.022 (3)	0.017 (3)	0.008 (2)	0.010 (3)	0.001 (2)	0.001 (2)
O6	0.026 (4)	0.026 (3)	0.015 (3)	0.014 (3)	0.003 (3)	0.004 (2)

O7	0.022 (3)	0.020 (3)	0.019 (3)	0.005 (3)	0.000 (3)	0.006 (2)
O8	0.030 (4)	0.022 (3)	0.022 (3)	0.013 (3)	-0.001 (3)	0.009 (2)
O9	0.011 (3)	0.017 (3)	0.017 (3)	0.000 (2)	-0.003 (2)	0.007 (2)
O10	0.024 (3)	0.023 (3)	0.019 (3)	-0.013 (3)	-0.007 (3)	0.008 (2)
O11	0.022 (3)	0.013 (3)	0.024 (3)	0.001 (3)	0.011 (3)	-0.004 (2)
O12	0.011 (3)	0.029 (3)	0.012 (2)	0.003 (3)	0.004 (2)	0.007 (2)
O13	0.038 (5)	0.063 (6)	0.014 (3)	0.035 (4)	-0.005 (3)	0.001 (3)
O14	0.015 (3)	0.029 (3)	0.012 (2)	-0.008 (3)	-0.005 (2)	0.008 (2)
O15	0.009 (3)	0.014 (3)	0.046 (4)	0.003 (2)	-0.011 (3)	0.002 (3)
O16	0.014 (3)	0.008 (2)	0.020 (3)	0.003 (2)	0.001 (2)	0.005 (2)
O17	0.019 (3)	0.020 (3)	0.006 (2)	0.006 (2)	0.006 (2)	0.006 (2)
O18	0.022 (3)	0.025 (3)	0.015 (2)	0.006 (3)	0.005 (2)	-0.005 (2)
O191	0.018 (5)	0.011 (4)	0.021 (4)	0.004 (4)	0.012 (4)	0.002 (3)
O192	0.018 (5)	0.011 (4)	0.021 (4)	0.004 (4)	0.012 (4)	0.002 (3)
O20	0.028 (8)	0.066 (11)	0.010 (5)	0.026 (8)	0.007 (5)	0.020 (6)

Geometric parameters (Å, °)

La1—O10 ⁱ	2.400 (6)	Te2—O191	2.156 (11)
La1—O6	2.435 (7)	Te2—O192	2.488 (14)
La1—O191 ⁱ	2.448 (12)	Te3—O15	1.841 (6)
La1—O16	2.485 (6)	Te3—O2	1.861 (7)
La1—O3	2.502 (6)	Te3—O4 ^{ix}	1.919 (6)
La1—O7	2.539 (6)	Te3—O13	2.496 (10)
La1—O11 ⁱ	2.647 (6)	Te4—O16	1.863 (6)
La1—O10	2.652 (7)	Te4—O17	1.871 (5)
La1—O192 ⁱ	2.706 (15)	Te4—O18	1.877 (7)
La2—O9	2.345 (6)	Te5—O13	1.831 (9)
La2—O17	2.400 (6)	Te5—O7	1.845 (7)
La2—O11	2.441 (6)	Te5—O20 ^{vi}	1.936 (13)
La2—O9 ⁱⁱ	2.528 (7)	Te5—O192 ⁱ	1.945 (15)
La2—O1 ⁱ	2.531 (6)	Te6—O5 ^x	1.859 (7)
La2—O8	2.643 (6)	Te6—O14 ⁱ	1.866 (5)
La2—O14	2.651 (6)	Te6—O12	1.883 (6)
La2—O6 ⁱ	2.985 (7)	O1—Te2 ^{viii}	2.032 (7)
La3—O15	2.447 (6)	O1—La5 ^{2xi}	2.131 (9)
La3—O18	2.454 (6)	O1—La5 ^{1xi}	2.446 (7)
La3—O12 ⁱⁱⁱ	2.456 (6)	O1—La2 ⁱ	2.531 (6)
La3—O5 ^{iv}	2.477 (6)	O2—La4 ^{xii}	2.453 (8)
La3—O4 ⁱⁱ	2.489 (7)	O2—La3 ^{xii}	2.655 (7)
La3—O4 ^v	2.557 (7)	O3—La4 ^{xii}	2.398 (5)
La3—O12 ^{vi}	2.633 (5)	O4—Te3 ^{xiii}	1.919 (6)
La3—O2 ^{iv}	2.655 (7)	O4—La3 ⁱⁱ	2.489 (7)
La4—O3 ^{iv}	2.398 (5)	O4—La3 ^{xiv}	2.557 (7)
La4—O2 ^{iv}	2.453 (8)	O5—Te6 ⁱⁱⁱ	1.859 (7)
La4—O191 ⁱ	2.476 (11)	O5—La3 ^{xii}	2.477 (6)
La4—O16	2.513 (7)	O5—La5 ^{1xii}	2.612 (6)
La4—O7 ^{iv}	2.516 (7)	O5—La5 ^{2xii}	2.902 (8)

La4—O13	2.522 (7)	O6—Te2 ^{viii}	1.866 (6)
La4—O192 ⁱ	2.556 (15)	O6—La2 ⁱ	2.985 (7)
La4—O20	2.626 (13)	O7—La4 ^{xii}	2.516 (7)
La4—O15	2.733 (6)	O8—La51 ^{xii}	2.589 (7)
La4—O18	2.995 (7)	O8—La52 ^{xii}	2.829 (9)
La51—O9 ^{iv}	2.393 (6)	O9—La52 ^{xii}	2.023 (7)
La51—O9 ⁱⁱ	2.420 (7)	O9—La52 ⁱⁱ	2.107 (9)
La51—O1 ^{vii}	2.446 (7)	O9—La51 ^{xii}	2.393 (6)
La51—O14 ⁱⁱ	2.521 (6)	O9—La51 ⁱⁱ	2.420 (7)
La51—O17	2.565 (7)	O9—La2 ⁱⁱ	2.528 (7)
La51—O8 ^{iv}	2.589 (7)	O10—La1 ⁱ	2.400 (6)
La51—O5 ^{iv}	2.612 (6)	O11—La1 ⁱ	2.647 (6)
La51—O18	2.763 (7)	O12—La3 ^x	2.456 (6)
La52—O9 ^{iv}	2.023 (7)	O12—La3 ^{vi}	2.633 (5)
La52—O9 ⁱⁱ	2.107 (9)	O14—Te6 ⁱ	1.866 (5)
La52—O1 ^{vii}	2.131 (9)	O14—La51 ⁱⁱ	2.521 (6)
La52—O14 ⁱⁱ	2.604 (7)	O14—La52 ⁱⁱ	2.604 (7)
La52—O8 ^{iv}	2.829 (9)	O191—O192	0.808 (16)
La52—O17	2.872 (8)	O191—La1 ⁱ	2.448 (12)
La52—O5 ^{iv}	2.902 (8)	O191—La4 ⁱ	2.476 (11)
Te1—O10	1.861 (6)	O192—Te5 ⁱ	1.945 (15)
Te1—O8	1.864 (7)	O192—La4 ⁱ	2.556 (15)
Te1—O3	1.872 (6)	O192—La1 ⁱ	2.706 (15)
Te2—O11	1.857 (7)	O20—O20 ^{xv}	1.75 (4)
Te2—O6 ^{viii}	1.866 (6)	O20—Te5 ^{vi}	1.936 (13)
Te2—O1 ^{viii}	2.032 (7)		
O10 ⁱ —La1—O6	100.8 (2)	O9 ⁱⁱ —La51—O5 ^{iv}	159.6 (2)
O10 ⁱ —La1—O191 ⁱ	97.2 (3)	O1 ^{vii} —La51—O5 ^{iv}	71.5 (2)
O6—La1—O191 ⁱ	121.3 (3)	O14 ⁱⁱ —La51—O5 ^{iv}	94.0 (2)
O10 ⁱ —La1—O16	99.0 (2)	O17—La51—O5 ^{iv}	122.32 (18)
O6—La1—O16	156.5 (2)	O8 ^{iv} —La51—O5 ^{iv}	94.0 (2)
O191 ⁱ —La1—O16	68.0 (3)	O9 ^{iv} —La51—O18	149.6 (2)
O10 ⁱ —La1—O3	123.0 (2)	O9 ⁱⁱ —La51—O18	125.3 (2)
O6—La1—O3	87.4 (2)	O1 ^{vii} —La51—O18	126.6 (2)
O191 ⁱ —La1—O3	126.1 (3)	O14 ⁱⁱ —La51—O18	75.5 (2)
O16—La1—O3	71.2 (2)	O17—La51—O18	58.70 (18)
O10 ⁱ —La1—O7	168.4 (2)	O8 ^{iv} —La51—O18	79.75 (19)
O6—La1—O7	75.5 (2)	O5 ^{iv} —La51—O18	64.02 (19)
O191 ⁱ —La1—O7	76.1 (3)	O9 ^{iv} —La52—O9 ⁱⁱ	86.2 (3)
O16—La1—O7	87.4 (2)	O9 ^{iv} —La52—O1 ^{vii}	86.6 (3)
O3—La1—O7	68.2 (2)	O9 ⁱⁱ —La52—O1 ^{vii}	108.8 (4)
O10 ⁱ —La1—O11 ⁱ	73.2 (2)	O9 ^{iv} —La52—O14 ⁱⁱ	156.7 (4)
O6—La1—O11 ⁱ	73.3 (2)	O9 ⁱⁱ —La52—O14 ⁱⁱ	76.7 (3)
O191 ⁱ —La1—O11 ⁱ	59.6 (3)	O1 ^{vii} —La52—O14 ⁱⁱ	84.1 (3)
O16—La1—O11 ⁱ	125.0 (2)	O9 ^{iv} —La52—O8 ^{iv}	71.1 (3)
O3—La1—O11 ⁱ	157.5 (2)	O9 ⁱⁱ —La52—O8 ^{iv}	106.8 (3)
O7—La1—O11 ⁱ	95.2 (2)	O1 ^{vii} —La52—O8 ^{iv}	136.2 (3)

O10 ⁱ —La1—O10	63.2 (3)	O14 ⁱⁱ —La52—O8 ^{iv}	128.9 (3)
O6—La1—O10	86.3 (2)	O9 ^{iv} —La52—O17	117.3 (3)
O191 ⁱ —La1—O10	149.8 (3)	O9 ⁱⁱ —La52—O17	69.9 (3)
O16—La1—O10	91.4 (2)	O1 ^{vii} —La52—O17	155.5 (3)
O3—La1—O10	61.16 (18)	O14 ⁱⁱ —La52—O17	71.7 (2)
O7—La1—O10	126.7 (2)	O8 ^{iv} —La52—O17	62.9 (2)
O11 ⁱ —La1—O10	127.04 (19)	O9 ^{iv} —La52—O5 ^{iv}	110.9 (3)
O10 ⁱ —La1—O192 ⁱ	113.7 (4)	O9 ⁱⁱ —La52—O5 ^{iv}	162.5 (3)
O6—La1—O192 ⁱ	111.4 (4)	O1 ^{vii} —La52—O5 ^{iv}	70.1 (3)
O191 ⁱ —La1—O192 ⁱ	17.1 (4)	O14 ⁱⁱ —La52—O5 ^{iv}	85.8 (2)
O16—La1—O192 ⁱ	71.3 (3)	O8 ^{iv} —La52—O5 ^{iv}	83.1 (2)
O3—La1—O192 ⁱ	115.1 (3)	O17—La52—O5 ^{iv}	103.5 (2)
O7—La1—O192 ⁱ	59.1 (4)	O10—Te1—O8	100.6 (3)
O11 ⁱ —La1—O192 ⁱ	63.8 (3)	O10—Te1—O3	89.4 (3)
O10—La1—O192 ⁱ	162.1 (4)	O8—Te1—O3	96.2 (3)
O10 ⁱ —La1—Te1	93.63 (16)	O11—Te2—O6 ^{viii}	102.3 (3)
O9—La2—O17	99.5 (2)	O11—Te2—O1 ^{viii}	95.2 (3)
O9—La2—O11	106.8 (2)	O6 ^{viii} —Te2—O1 ^{viii}	86.7 (3)
O17—La2—O11	122.0 (2)	O11—Te2—O191	78.0 (4)
O9—La2—O9 ⁱⁱ	72.4 (3)	O6 ^{viii} —Te2—O191	90.4 (4)
O17—La2—O9 ⁱⁱ	72.6 (2)	O1 ^{viii} —Te2—O191	171.9 (4)
O11—La2—O9 ⁱⁱ	164.7 (2)	O11—Te2—O192	79.9 (4)
O9—La2—O1 ⁱ	128.0 (2)	O6 ^{viii} —Te2—O192	108.0 (4)
O17—La2—O1 ⁱ	100.2 (2)	O1 ^{viii} —Te2—O192	165.2 (4)
O11—La2—O1 ⁱ	102.3 (2)	O191—Te2—O192	18.3 (4)
O9 ⁱⁱ —La2—O1 ⁱ	68.6 (2)	O15—Te3—O2	101.3 (3)
O9—La2—O8	70.7 (2)	O15—Te3—O4 ^{ix}	99.7 (3)
O17—La2—O8	67.6 (2)	O2—Te3—O4 ^{ix}	88.2 (3)
O11—La2—O8	73.9 (2)	O15—Te3—O13	73.6 (3)
O9 ⁱⁱ —La2—O8	118.8 (2)	O2—Te3—O13	89.1 (3)
O1 ⁱ —La2—O8	160.4 (2)	O4 ^{ix} —Te3—O13	172.1 (2)
O9—La2—O14	72.04 (19)	O16—Te4—O17	99.0 (3)
O17—La2—O14	161.3 (2)	O16—Te4—O18	94.0 (3)
O11—La2—O14	76.7 (2)	O17—Te4—O18	88.6 (3)
O9 ⁱⁱ —La2—O14	88.8 (2)	O13—Te5—O7	101.0 (4)
O1 ⁱ —La2—O14	74.1 (2)	O13—Te5—O20 ^{vi}	95.8 (6)
O8—La2—O14	122.3 (2)	O7—Te5—O20 ^{vi}	100.5 (5)
O9—La2—O6 ⁱ	173.5 (2)	O13—Te5—O192 ⁱ	80.4 (5)
O17—La2—O6 ⁱ	82.1 (2)	O7—Te5—O192 ⁱ	86.2 (5)
O11—La2—O6 ⁱ	67.3 (2)	O20 ^{vi} —Te5—O192 ⁱ	172.9 (6)
O9 ⁱⁱ —La2—O6 ⁱ	114.1 (2)	O5 ^x —Te6—O14 ⁱ	96.7 (3)
O1 ⁱ —La2—O6 ⁱ	57.4 (2)	O5 ^x —Te6—O12	99.5 (3)
O8—La2—O6 ⁱ	104.5 (2)	O14 ⁱ —Te6—O12	100.2 (3)
O14—La2—O6 ⁱ	108.17 (17)	Te2 ^{viii} —O1—La52 ^{xi}	140.8 (4)
O15—La3—O18	68.9 (2)	Te2 ^{viii} —O1—La51 ^{xi}	139.5 (3)
O15—La3—O12 ⁱⁱⁱ	87.2 (2)	La52 ^{xi} —O1—La51 ^{xi}	11.06 (15)
O18—La3—O12 ⁱⁱⁱ	83.6 (2)	Te2 ^{viii} —O1—La2 ⁱ	113.0 (3)
O15—La3—O5 ^{iv}	137.5 (2)	La52 ^{xi} —O1—La2 ⁱ	100.1 (3)

O18—La3—O5 ^{iv}	70.7 (2)	La51 ^{xi} —O1—La2 ⁱ	105.8 (2)
O12 ⁱⁱⁱ —La3—O5 ^{iv}	100.8 (2)	Te3—O2—La4 ^{xii}	133.6 (4)
O15—La3—O4 ⁱⁱ	150.80 (19)	Te3—O2—La3 ^{xii}	104.2 (3)
O18—La3—O4 ⁱⁱ	134.4 (2)	La4 ^{xii} —O2—La3 ^{xii}	101.3 (3)
O12 ⁱⁱⁱ —La3—O4 ⁱⁱ	80.0 (2)	Te1—O3—La4 ^{xii}	134.1 (3)
O5 ^{iv} —La3—O4 ⁱⁱ	71.1 (2)	Te1—O3—La1	107.3 (2)
O15—La3—O4 ^v	103.2 (2)	La4 ^{xii} —O3—La1	113.3 (2)
O18—La3—O4 ^v	134.4 (2)	Te3 ^{xiii} —O4—La3 ⁱⁱ	139.3 (3)
O12 ⁱⁱⁱ —La3—O4 ^v	141.94 (19)	Te3 ^{xiii} —O4—La3 ^{xiv}	106.1 (3)
O5 ^{iv} —La3—O4 ^v	95.7 (2)	La3 ⁱⁱ —O4—La3 ^{xiv}	106.7 (2)
O4 ⁱⁱ —La3—O4 ^v	73.3 (2)	Te6 ⁱⁱⁱ —O5—La3 ^{xii}	121.3 (3)
O15—La3—O12 ^{vi}	75.3 (2)	Te6 ⁱⁱⁱ —O5—La51 ^{xii}	119.3 (3)
O18—La3—O12 ^{vi}	140.1 (2)	La3 ^{xii} —O5—La51 ^{xii}	109.6 (3)
O12 ⁱⁱⁱ —La3—O12 ^{vi}	77.4 (2)	Te6 ⁱⁱⁱ —O5—La52 ^{xii}	109.8 (3)
O5 ^{iv} —La3—O12 ^{vi}	147.1 (2)	La3 ^{xii} —O5—La52 ^{xii}	117.1 (3)
O4 ⁱⁱ —La3—O12 ^{vi}	76.3 (2)	La51 ^{xii} —O5—La52 ^{xii}	9.51 (11)
O4 ^v —La3—O12 ^{vi}	70.38 (19)	Te2 ^{viii} —O6—La1	131.9 (3)
O15—La3—O2 ^{iv}	72.9 (2)	Te2 ^{viii} —O6—La2 ⁱ	101.1 (3)
O18—La3—O2 ^{iv}	74.6 (2)	La1—O6—La2 ⁱ	100.1 (2)
O12 ⁱⁱⁱ —La3—O2 ^{iv}	154.5 (2)	Te5—O7—La4 ^{xii}	128.2 (3)
O5 ^{iv} —La3—O2 ^{iv}	84.6 (2)	Te5—O7—La1	112.1 (3)
O4 ⁱⁱ —La3—O2 ^{iv}	124.9 (2)	La4 ^{xii} —O7—La1	108.2 (2)
O4 ^v —La3—O2 ^{iv}	60.6 (2)	Te1—O8—La51 ^{xii}	120.8 (3)
O12 ^{vi} —La3—O2 ^{iv}	111.4 (2)	Te1—O8—La2	129.5 (3)
O15—La3—Te3 ^{iv}	84.65 (18)	La51 ^{xii} —O8—La2	100.7 (2)
O18—La3—Te3 ^{iv}	104.67 (17)	Te1—O8—La52 ^{xii}	127.0 (4)
O12 ⁱⁱⁱ —La3—Te3 ^{iv}	165.27 (13)	La51 ^{xii} —O8—La52 ^{xii}	10.27 (10)
O5 ^{iv} —La3—Te3 ^{iv}	93.53 (16)	La2—O8—La52 ^{xii}	91.0 (2)
O4 ⁱⁱ —La3—Te3 ^{iv}	101.55 (16)	La52 ^{xii} —O9—La52 ⁱⁱ	93.8 (3)
O4 ^v —La3—Te3 ^{iv}	30.83 (13)	La52 ^{xii} —O9—La2	126.6 (3)
O12 ^{vi} —La3—Te3 ^{iv}	88.70 (14)	La52 ⁱⁱ —O9—La2	108.6 (3)
O2 ^{iv} —La3—Te3 ^{iv}	30.10 (14)	La52 ^{xii} —O9—La51 ^{xii}	10.31 (16)
O3 ^{iv} —La4—O2 ^{iv}	87.2 (2)	La52 ⁱⁱ —O9—La51 ^{xii}	99.6 (3)
O3 ^{iv} —La4—O191 ⁱ	81.8 (3)	La2—O9—La51 ^{xii}	116.4 (3)
O2 ^{iv} —La4—O191 ⁱ	158.2 (3)	La52 ^{xii} —O9—La51 ⁱⁱ	101.2 (3)
O3 ^{iv} —La4—O16	71.8 (2)	La52 ⁱⁱ —O9—La51 ⁱⁱ	11.21 (15)
O2 ^{iv} —La4—O16	126.8 (2)	La2—O9—La51 ⁱⁱ	109.7 (2)
O191 ⁱ —La4—O16	67.2 (3)	La51 ^{xii} —O9—La51 ⁱⁱ	108.1 (3)
O3 ^{iv} —La4—O7 ^{iv}	70.2 (2)	La52 ^{xii} —O9—La2 ⁱⁱ	103.2 (3)
O2 ^{iv} —La4—O7 ^{iv}	88.0 (2)	La52 ⁱⁱ —O9—La2 ⁱⁱ	117.3 (3)
O191 ⁱ —La4—O7 ^{iv}	70.6 (3)	La2—O9—La2 ⁱⁱ	107.6 (3)
O16—La4—O7 ^{iv}	125.9 (2)	La51 ^{xii} —O9—La2 ⁱⁱ	107.5 (2)
O3 ^{iv} —La4—O13	153.1 (3)	La51 ⁱⁱ —O9—La2 ⁱⁱ	107.1 (2)
O2 ^{iv} —La4—O13	119.0 (2)	Te1—O10—La1 ⁱ	139.7 (3)
O191 ⁱ —La4—O13	75.2 (3)	Te1—O10—La1	102.0 (2)
O16—La4—O13	86.4 (3)	La1 ⁱ —O10—La1	116.8 (3)
O7 ^{iv} —La4—O13	113.6 (3)	Te2—O11—La2	138.5 (3)
O3 ^{iv} —La4—O192 ⁱ	100.2 (4)	Te2—O11—La1 ⁱ	111.5 (3)

O2 ^{iv} —La4—O192 ⁱ	159.8 (4)	La2—O11—La1 ⁱ	110.0 (3)
O191 ⁱ —La4—O192 ⁱ	18.4 (4)	Te6—O12—La3 ^x	140.4 (3)
O16—La4—O192 ⁱ	73.4 (4)	Te6—O12—La3 ^{vi}	117.0 (3)
O7 ^{iv} —La4—O192 ⁱ	77.0 (4)	La3 ^x —O12—La3 ^{vi}	102.6 (2)
O13—La4—O192 ⁱ	57.4 (4)	Te5—O13—Te3	133.3 (4)
O3 ^{iv} —La4—O20	129.1 (4)	Te5—O13—La4	113.8 (4)
O2 ^{iv} —La4—O20	71.6 (4)	Te3—O13—La4	104.4 (3)
O191 ⁱ —La4—O20	101.1 (5)	Te6 ⁱ —O14—La51 ⁱⁱ	149.0 (3)
O16—La4—O20	155.9 (3)	Te6 ⁱ —O14—La52 ⁱⁱ	157.7 (4)
O7 ^{iv} —La4—O20	63.5 (4)	La51 ⁱⁱ —O14—La52 ⁱⁱ	11.98 (12)
O13—La4—O20	70.0 (4)	Te6 ⁱ —O14—La2	112.9 (3)
O192 ⁱ —La4—O20	89.4 (5)	La51 ⁱⁱ —O14—La2	97.73 (17)
O3 ^{iv} —La4—O15	131.0 (2)	La52 ⁱⁱ —O14—La2	87.0 (2)
O2 ^{iv} —La4—O15	71.4 (2)	Te3—O15—La3	141.2 (3)
O191 ⁱ —La4—O15	129.5 (3)	Te3—O15—La4	119.0 (3)
O16—La4—O15	86.3 (2)	La3—O15—La4	99.34 (19)
O7 ^{iv} —La4—O15	147.7 (2)	Te4—O16—La1	137.7 (3)
O13—La4—O15	60.4 (3)	Te4—O16—La4	109.3 (3)
O192 ⁱ —La4—O15	115.1 (4)	La1—O16—La4	110.7 (2)
O20—La4—O15	85.9 (4)	Te4—O17—La2	133.5 (3)
O3 ^{iv} —La4—O18	73.59 (18)	Te4—O17—La51	105.0 (2)
O2 ^{iv} —La4—O18	68.6 (2)	La2—O17—La51	106.5 (2)
O191 ⁱ —La4—O18	125.1 (3)	Te4—O17—La52	112.6 (3)
O16—La4—O18	58.79 (19)	La2—O17—La52	97.1 (2)
O7 ^{iv} —La4—O18	137.49 (19)	La51—O17—La52	9.40 (11)
O13—La4—O18	108.8 (3)	Te4—O18—La3	135.8 (3)
O192 ⁱ —La4—O18	131.5 (4)	Te4—O18—La51	97.8 (3)
O20—La4—O18	132.5 (4)	La3—O18—La51	105.6 (2)
O15—La4—O18	57.66 (18)	Te4—O18—La4	92.0 (3)
O9 ^{iv} —La51—O9 ⁱⁱ	71.9 (3)	La3—O18—La4	92.5 (2)
La52—La51—O1 ^{vii}	49.1 (5)	La51—O18—La4	141.2 (2)
O9 ^{iv} —La51—O1 ^{vii}	72.2 (2)	O192—O191—Te2	104.8 (14)
O9 ⁱⁱ —La51—O1 ^{vii}	90.2 (2)	O192—O191—La1 ⁱ	99.9 (15)
La52—La51—O14 ⁱⁱ	92.8 (5)	Te2—O191—La1 ⁱ	108.9 (5)
O9 ^{iv} —La51—O14 ⁱⁱ	134.6 (2)	O192—O191—La4 ⁱ	86.4 (13)
O9 ⁱⁱ —La51—O14 ⁱⁱ	73.25 (19)	Te2—O191—La4 ⁱ	133.7 (6)
O1 ^{vii} —La51—O14 ⁱⁱ	79.9 (2)	La1 ⁱ —O191—La4 ⁱ	113.2 (4)
La52—La51—O17	119.8 (6)	O191—O192—Te5 ⁱ	165.3 (18)
O9 ^{iv} —La51—O17	115.9 (2)	O191—O192—Te2	56.9 (12)
O9 ⁱⁱ —La51—O17	71.7 (2)	Te5 ⁱ —O192—Te2	129.3 (7)
O1 ^{vii} —La51—O17	155.0 (2)	O191—O192—La4 ⁱ	75.2 (13)
O14 ⁱⁱ —La51—O17	78.4 (2)	Te5 ⁱ —O192—La4 ⁱ	108.3 (6)
La52—La51—O8 ^{iv}	111.1 (5)	Te2—O192—La4 ⁱ	115.3 (6)
O9 ^{iv} —La51—O8 ^{iv}	71.0 (2)	O191—O192—La1 ⁱ	63.0 (14)
O9 ⁱⁱ —La51—O8 ^{iv}	105.4 (2)	Te5 ⁱ —O192—La1 ⁱ	102.4 (6)
O1 ^{vii} —La51—O8 ^{iv}	132.6 (2)	Te2—O192—La1 ⁱ	92.3 (5)
O14 ⁱⁱ —La51—O8 ^{iv}	147.3 (2)	La4 ⁱ —O192—La1 ⁱ	102.7 (5)
O17—La51—O8 ^{iv}	70.5 (2)	O20 ^{xv} —O20—Te5 ^{vi}	95.3 (9)

La52—La51—O5 ^{iv}	117.6 (5)	O20 ^{xv} —O20—La4	133.2 (12)
O9 ^{iv} —La51—O5 ^{iv}	109.5 (2)	Te5 ^{vi} —O20—La4	120.3 (8)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$; (iii) $x, y-1, z$; (iv) $x+1, y, z$; (v) $x+1, y, z-1$; (vi) $-x+1, -y+1, -z$; (vii) $x+1, y-1, z$; (viii) $-x, -y+1, -z+1$; (ix) $x, y, z-1$; (x) $x, y+1, z$; (xi) $x-1, y+1, z$; (xii) $x-1, y, z$; (xiii) $x, y, z+1$; (xiv) $x-1, y, z+1$; (xv) $-x+2, -y+1, -z$.